

STIC Search Report

EIC 1700

STIC Database Tracking Number: 188873

TO: Michael Bernshteyn
Location: REM 10A34
Art Unit : 1713
May 12, 2006

Case Serial Number: 10/534388

From: Usha Shrestha
Location: EIC 1700
REMSSEN 4B28
Phone: 571/272-3519
usha.shrestha@uspto.gov

Search Notes



STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact *the EIC searcher* or contact:

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- I am an examiner in Workgroup: Example: 1713
- Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

- Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability)
- ☐ Results were not useful in determining patentability or understanding the invention

Comments:

Access DB# 188873**SEARCH REQUEST FORM**

Scientific and Technical Information Center

Requester's Full Name: MICHAEL BERNSTEIN Examiner #: 81515 Date: 05/03/06
Art Unit: 1713 Phone Number 30 272-2411 Serial Number: 10/534,308
Mail Box and Bldg/Room Location: RM. 10A34 Results Format Preferred (circle) PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Method for radical polymerization in the presence of
Inventors (please provide full names): Wolfgang Gaschler Chark Transire

Earliest Priority Filing Date: 12/03/2002

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please, try to find the regulator with the formulae (I), (II), (III) or (IV) according to claim 4.

Thank you
M. Bernstein

SCIENTIFIC REFERENCE BR
Sci & Tech Inf. Ctr.

MAY 5 REC.

Pat. & T.M. Office

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>WGL</u>	NA Sequence (#) _____	STN <u>701-87</u>
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>1</u>	Questel/Orbit _____
Date Searcher Picked Up: <u>5/12/06</u>	Bibliographic _____	Dr. Link _____
Date Completed: <u>5/12/06</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>120</u>	Fulltext _____	Sequence Systems _____
Clerical Prep Time: <u>30</u>	Patent Family _____	WWW/Internet _____
Online Time: <u>200</u>	Other _____	Other (specify) _____

IN THE CLAIMS

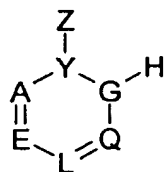
Please amend the claims as follows:

Claim 1 (Currently Amended): A process for free-radical polymerization in the presence of a regulator, ~~which comprises using, as wherein said~~ regulator comprises, a carbocyclic or heterocyclic ~~compounds~~ compound which ~~contain~~ comprises a leaving group in the allyl or heteroallyl position, or homoallyl or homoheteroallyl position, respectively, ~~where these compounds wherein said carbocyclic or heterocyclic compound,~~ following free-radical hydrogen abstraction, ~~form~~ forms an aromatic system with elimination of a free-radical leaving group.

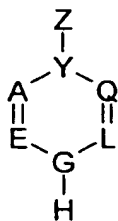
Claim 2 (Currently Amended): A The process as claimed in claim 1, wherein the aromatic system which forms is an optionally substituted phenyl, pyridine, pyridazine, pyrimidine, pyrazine, pyran, thiopyran, pyrrole, pyrazole, imidazole, furan, oxazole, isoxazole, thiophene, thiazol or isothiazol.

Claim 3 (Currently Amended): A The process as claimed in claim 1, wherein the leaving group is a carboxylate, silyl, sulfonyl, aryl, benzyl, allyl or alkyl group.

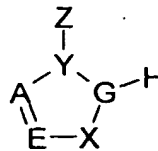
Claim 4 (Currently Amended): A The process as claimed in ~~claims 1 to 3~~ claim 1, wherein the regulator ~~chosen~~ is at least one compound from the formulae (I), (II), (III) or (IV)



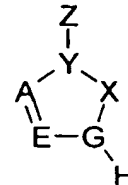
(I)



(II)



(III)



(IV)

in which

A is C-R¹, N,

E is C-R², N,

L is C-R³, N,

Q is C-R⁴, N,

where

R¹-R⁴ independently of one another are hydrogen, C₁-C₁₀-alkyl, C₁-C₁₀-alkoxy, C₁-C₁₀-alkylamino, C₂-C₂₀-dialkylamino, C₁-C₁₀-alkylcarbonyl, C₁-C₁₀-alkylsulfonyl, C₂-C₁₀-alkenyl, C₂-C₁₀-alkynyl, in which at least two of the radicals R¹-R⁴ may be joined together to give a 3- to 8-membered ring,

G is C-R⁵, N,

where R⁵ is hydrogen, C₁-C₁₀-alkyl,

X is O, N-R⁶, S,

where R⁶ is hydrogen, C₁-C₁₀-alkoxy, C₁-C₁₀-alkylamino, C₂-C₂₀-dialkylamino, C₁-C₁₀-alkylcarbonyl, C₁-C₁₀-alkylsulfonyl,

Y is C-R⁷, N,

where R⁷ is hydrogen, carboxyl, C₁-C₁₀-alkyl, C₁-C₁₀-alkoxy, C₁-C₁₀-alkylcarbonyl, C₁-C₁₀-alkoxycarbonyl, C₁-C₁₀-alkylaminocarbonyl, C₂-C₂₀-dialkylaminocarbonyl, C₁-C₁₀-alkylcarbonyloxy, C₁-C₁₀-alkylcarbonylamino, C₁-C₁₀-alkylsulfonyl, C₁-C₁₀-alkoxysulfonyl, C₁-C₁₀-alkylaminosulfonyl, C₂-C₂₀-dialkylaminosulfonyl, C₁-C₁₀-acyl, C₂-C₁₀-alkenyl, C₃-C₁₀-alkenyloxy, C₂-C₁₀-alkenylcarbonyl, C₃-C₁₀-alkenyloxycarbonyl, C₃-C₁₀-alkenylaminocarbonyl, C₂-C₁₀-alkenylcarbonyloxy, C₂-C₁₀-alkenylcarbonylamino, C₂-C₁₀-alkenylsulfonyl, C₃-C₁₀-alkenyloxysulfonyl, C₃-C₁₀-alkenylaminosulfonyl, C₂-C₁₀-alkynyl, C₃-C₁₀-alkynyloxy, C₂-C₁₀-alkynylcarbonyl, C₃-C₁₀-alkynyloxycarbonyl, C₃-C₁₀-alkynylaminocarbonyl, C₂-C₁₀-

alkynylcarbonyloxy, C₂-C₁₀-alkynylcarbonylamino, C₂-C₁₀-alkynylsulfonyl, C₃-C₁₀-alkynyloxysulfonyl, C₃-C₁₀-alkynylaminosulfonyl, C₃-C₁₂-cycloalkyl, C₃-C₁₂-cycloalkoxy, C₃-C₁₂-cycloalkylcarbonyl, C₃-C₁₂-cycloalkoxycarbonyl, C₃-C₁₂-cycloalkylaminocarbonyl, C₃-C₁₂-cycloalkylcarbonyloxy, C₃-C₁₂-cycloalkylcarbonylamino, C₃-C₁₂-cycloalkylsulfonyl, C₃-C₁₂-cycloalkoxysulfonyl, C₃-C₁₂-cycloalkylaminosulfonyl, aryl, aryloxy, arylcarbonyl, aryloxy carbonyl, arylaminocarbonyl, arylcarbonyloxy, arylcarbonylamino, arylsulfonyl, aryloxysulfonyl, arylaminosulfonyl,

Z is COOR⁸, SiR⁹R¹⁰R¹¹, SO₂R¹², aryl, optionally substituted benzyl, C₃-C₁₀-2-alken-1-yl, R¹³

where

R⁸, R¹³ are C₁-C₁₀-alkyl,

R⁹-R¹¹ independently of one another are hydrogen, C₁-C₁₀-alkyl, in

which two of the radicals R⁹-R¹¹ may be joined together to give a 3- to 8-membered ring, R¹² is hydrogen, C₁-C₁₀-alkyl,

with the proviso that a maximum of 2 heteroatoms are in the ring of the heterocyclic compound.

Claim 5 (Currently Amended): A The process as claimed in ~~claims 1 to 4~~ claim 1, wherein the regulator used is cyclohexadienecarboxylic acid optionally substituted by C₁-C₄-alkyl radicals as R⁷, methyl cyclohexadienecarboxylate, ethyl cyclohexadienecarboxylate, dihydrofurancarboxylic acid, methyl dihydrofurancarboxylate and/or ethyl dihydrofurancarboxylate.

Claim 6 (Currently Amended): A The process as claimed in ~~claims 1 to 5~~ claim 1, wherein the regulator used is methyl 1-methyl-2,5-cyclohexadiene-1-carboxylate, 1-

=> fil reg
FILE 'REGISTRY' ENTERED AT 13:30:52 ON 12 MAY 2006

=> d his ful

FILE 'HCAPLUS' ENTERED AT 10:17:27 ON 12 MAY 2006

L1 1 SEA ABB=ON PLU=ON US20060058478/PN

FILE 'REGISTRY' ENTERED AT 10:17:56 ON 12 MAY 2006

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OR 25212-88-8/BI OR 31689-39-1/BI OR 380883-30-7/BI OR
52457-02-0/BI OR 52457-04-2/BI OR 59034-54-7/BI OR
9003-39-8/BI OR 9003-53-6/BI)
L3 STR
L4 SCR 2043
L5 50 SEA SSS SAM L3 AND L4
L6 SCR 1841
L7 50 SEA SSS SAM L3 AND L4 NOT L6
L8 SCR 2127
L9 50 SEA SSS SAM L3 AND L4 NOT (L6 OR L8)
L10 SCR 1840
L11 50 SEA SSS SAM L3 AND L4 NOT (L10 OR L8)
L12 STR L3
L13 50 SEA SSS SAM L12 NOT (L10 OR L8)
L14 STR L12
L15 36 SEA SSS SAM L14 NOT (L10 OR L8)
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L18 32 SEA SSS SAM L14 NOT (L8 OR L10 OR L17)
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L21 SCR 1839
L22 8 SEA SSS SAM L19 NOT (L21 OR L8 OR L17)
L23 SCR 1695 OR 1549 OR 1795 OR 1312 OR 1482 OR 1048 OR 180
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L35 10 SEA SSS SAM L34
L36 STR L34
L37 1 SEA ABB=ON PLU=ON 59034-54-7/RN

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L38 16 SEA ABB=ON PLU=ON L37

FILE 'REGISTRY' ENTERED AT 12:54:07 ON 12 MAY 2006

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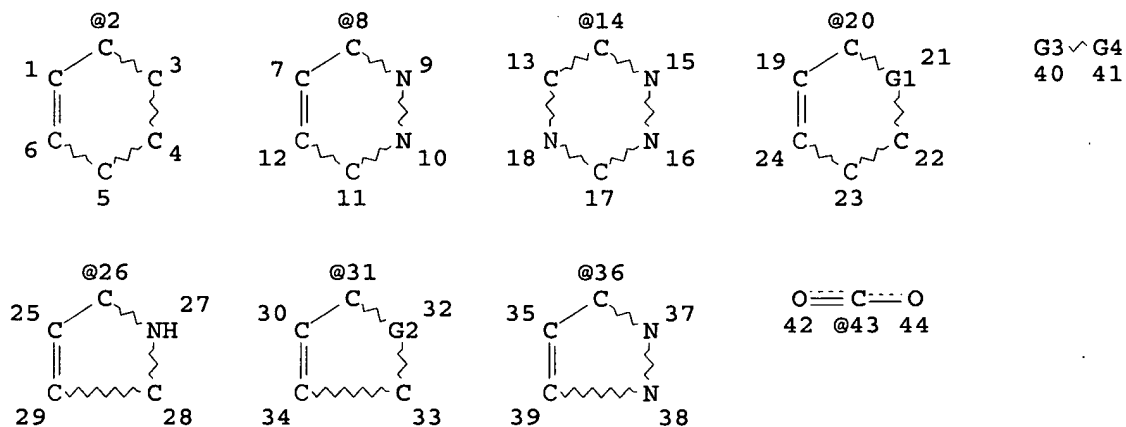
SAV L45 BER388/A

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 L49 16 SEA ABB=ON PLU=ON L38 AND L46
 L50 3537 SEA ABB=ON PLU=ON L46 AND PREP/RL
 L51 28 SEA ABB=ON PLU=ON L50 AND REGULATOR?
 L52 86 SEA ABB=ON PLU=ON L50 AND (PLASTIC? OR POLYMER?)/SC,S
 X
 L53 52 SEA ABB=ON PLU=ON L52 AND P/DT
 L54 47 SEA ABB=ON PLU=ON L53 AND (1907-2002)/PRY,AY
 L55 34 SEA ABB=ON PLU=ON L52 NOT L53
 L56 26 SEA ABB=ON PLU=ON L55 NOT (2003-2006)/PY
 L57 73 SEA ABB=ON PLU=ON L54 OR L56
 L58 5 SEA ABB=ON PLU=ON L57 AND RADIC?
 L59 73 SEA ABB=ON PLU=ON L57 OR L58
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 L61 0 SEA ABB=ON PLU=ON L60 AND P/DT
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=> d que 163

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 L21 SCR 1839
 L43 STR



VAR G1=O/N
 VAR G2=N/O
 VAR G3=20/14/8/2/26/31/36
 VAR G4=43/SI/SO2
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 44

STEREO ATTRIBUTES: NONE

L45 5427 SEA FILE=REGISTRY SSS FUL L43 NOT (L8 OR L17 OR L21)
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 POLYMER?)/SC,SX
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 L56 26 SEA FILE=HCAPLUS ABB=ON PLU=ON L55 NOT (2003-2006)/PY
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 L58 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L57 AND RADIC?
 L59 73 SEA FILE=HCAPLUS ABB=ON PLU=ON L57 OR L58
 L63 50 SEA FILE=HCAPLUS ABB=ON PLU=ON L59 AND POLYMERI?

=> fil hcap

FILE 'HCAPLUS' ENTERED AT 13:31:10 ON 12 MAY 2006

=> d l63 1-50 ibib abs hitstr hitind

L63 ANSWER 1 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:492253 HCAPLUS

DOCUMENT NUMBER: 141:54782

TITLE: **Radical polymerization in**
 presence of cyclohexa-2,5-dienecarboxylates as
polymerization regulators

PATENT ASSIGNEE(S): BASF AG, Germany

SOURCE: Ger. Offen., 15 pp.

CODEN: GWXXBX

DOCUMENT TYPE: **Patent**

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10256617	A1	20040617	DE 2002-10256617	2002 1203
WO 2004050717	A2	20040617	WO 2003-EP13489	2003 1201
WO 2004050717	A3	20040819		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY,				

CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
 NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA,
 GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003288203 A1 20040623 AU 2003-288203 2003
 1201

EP 1569965 A2 20050907 EP 2003-780091 2003
 1201

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
 MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ,
 EE, HU, SK

BR 2003016440 A 20051011 BR 2003-16440 2003
 1201

US 2006058478 A1 20060316 US 2005-534388 2005
 0509

PRIORITY APPLN. INFO.: DE 2002-10256617 A 2002
 1203

WO 2003-EP13489 W 2003
 1201

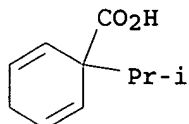
AB **Radical polymerization** is carried out in the presence of a carbocyclic or heterocyclic compound having a leaving groups in (homo)allyl or (homo)heteroallyl position which, after **radical H-abstraction**, forms an aromatic system with simultaneous cleavage of **radical** leaving group that starts a new free-**radical** chain. For example, acrylic acid-butadiene-styrene copolymer was prepared by **radical emulsion polymerization** of the monomers in the presence of 1-benzyl-2,5-cyclohexadiene-1-carboxylic acid as **polymerization** regulator.

IT 31689-39-1 52457-02-0 59034-54-7
 245672-30-4 380883-30-7

(**radical polymerization** in presence of cyclohexadienecarboxylates as **polymerization** regulators)

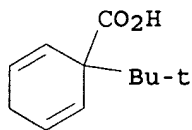
RN 31689-39-1 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1-methylethyl)- (9CI)
 (CA INDEX NAME)

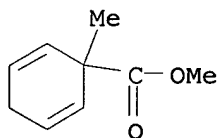


RN 52457-02-0 HCAPLUS

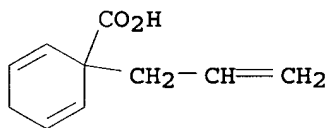
CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1,1-dimethylethyl)- (9CI)
 (CA INDEX NAME)



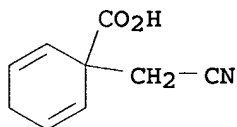
RN 59034-54-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
 (6CI, 9CI) (CA INDEX NAME)



RN 245672-30-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(2-propenyl)- (9CI) (CA
 INDEX NAME)



RN 380883-30-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(cyanomethyl)- (9CI) (CA
 INDEX NAME)



IC ICM C08F002-38
 ICS C08F212-08
 CC 35-2 (Chemistry of Synthetic High Polymers)
 ST **radical polymn** regulator
 benzylcyclohexadienecarboxylic acid
 IT **Polymerization** catalysts
 (radical; radical polymerization in
 presence of cyclohexadienecarboxylates as polymerization
 regulators)
 IT 31689-39-1 52457-02-0 52457-04-2
 59034-54-7 245672-30-4 380883-30-7
 (radical polymerization in presence of
 cyclohexadienecarboxylates as polymerization regulators)
 IT 9003-39-8P, N-Vinylpyrrolidone polymer 9003-53-6P, Polystyrene
 25085-39-6P, Acrylic acid-Butadiene-Styrene copolymer
 25212-88-8P, Ethyl acrylate-Methacrylic acid copolymer

(radical polymerization in presence of
cyclohexadienecarboxylates as polymerization regulators)

L63 ANSWER 2 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:477938 HCAPLUS

DOCUMENT NUMBER: 137:311838

TITLE: Synthesis of new membrane materials
incorporating tetrapyrrolic macrocycles.
Study of facilitated transport of the alkali
metals Li⁺, Na⁺ and K⁺

AUTHOR(S): Malek, Fouad; Persin, Michel; Ramdani,
Abdelkrim; Sarrazin, Jean; Zidane, Ismail

CORPORATE SOURCE: Laboratoire de Chimie Organique Physique,
Faculte des Sciences, Universite Mohamed
Premier, Oujda, 60 000, Morocco

SOURCE: New Journal of Chemistry (2002), 26(7),
876-882

CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

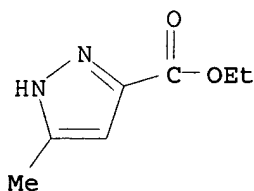
LANGUAGE: French

AB New macrocyclic ligands with two functionalized lateral arms were
synthesized. Their structures differ by the size of the
macrocyclic cavity. The membrane materials were obtained by
photopolymerization of formulations that contain the active monomer
spread on a polyacrylonitrile support. The facilitated transport
and the extraction power of alkaline metals (Li⁺, Na⁺ and K⁺) through the
synthesized membranes were reported. We have determined both the
diffusion flow of different cations and the selectivity of the
prepared membranes towards each cation.

IT 4027-57-0, 3-Ethoxycarbonyl-5-methylpyrazole
(starting material in monomer synthesis; synthesis of membrane
materials incorporating tetrapyrrolic macrocycles and their
performance in facilitated transport of Li⁺, Na⁺, K⁺)

RN 4027-57-0 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-methyl-, ethyl ester (9CI) (CA
INDEX NAME)



CC 38-3 (Plastics Fabrication and Uses)

Section cross-reference(s): 35

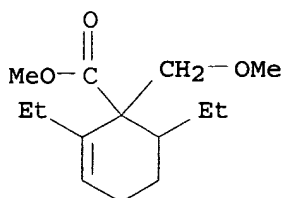
ST tetrapyrrolic macrocycle methacrylate synthesis photochem
polymn membrane material; alkali metal ion transport
tetrapyrrolic macrocycle polymethacrylate composite membrane

IT 156-87-6, 3-Aminopropanol 4027-57-0,
3-Ethoxycarbonyl-5-methylpyrazole
(starting material in monomer synthesis; synthesis of membrane
materials incorporating tetrapyrrolic macrocycles and their
performance in facilitated transport of Li⁺, Na⁺, K⁺)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE

IN THE RE FORMAT

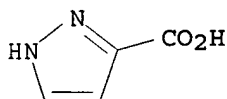
L63 ANSWER 3 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2002:125044 HCAPLUS
 DOCUMENT NUMBER: 137:6423
 TITLE: Synthesis and evaluation of
 1,3-diethyl-2,2-dimethoxymethylcyclohexane, an
 external electron donor in Ziegler-Natta
 catalysis
 AUTHOR(S): Grison, Claude; Batt-Coutrot, Delphine;
 Malinge, Jean; Saudemont, Thierry; Coutrot,
 Philippe
 CORPORATE SOURCE: Lab. de Chimie Organique Biomoleculaire, FR
 CNRS 1742, UMR 7565, Inst. Nanceien de Chimie
 Mol., Univ. Henri-Poincare,
 Vandoeuvre-les-Nancy, 54506, Fr.
 SOURCE: Comptes Rendus de l'Academie des Sciences,
 Serie IIC: Chimie (2001), 4(12), 893-898
 CODEN: CASCEN; ISSN: 1387-1609
 PUBLISHER: Editions Scientifiques et Medicales Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The first synthesis of 1,3 diethyl-2,2-dimethoxymethylcyclohexane
 starting from the easily available Me 6-ethyl-2-
 oxocyclohexanecarboxylate via a process involving the building up
 of a fourfold carbon by a regiospecific alkylation of a silyl enol
 ether and the introduction of the Et substituent by a carbanionic
 approach is described. The behavior of 1,3-di-Et
 2,2--diethoxymethylcyclohexane as external electron donor in high
 activity supported Ziegler-Natta catalyst is studied. The results
 presented show that this new donor allows the synthesis of
 polypropylene with a good isotacticity.
 IT 432551-37-6P
 (synthesis and evaluation of 1,3-diethyl-2,2-
 dimethoxymethylcyclohexane as external electron donor in
 Ziegler-Natta catalysis)
 RN 432551-37-6 HCAPLUS
 CN 2-Cyclohexene-1-carboxylic acid, 2,6-diethyl-1-(methoxymethyl)-,
 methyl ester (9CI) (CA INDEX NAME)



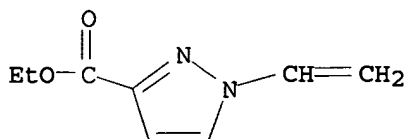
CC 35-3 (Chemistry of Synthetic High Polymers)
 IT Polymerization catalysts
 (Ziegler-Natta; synthesis and evaluation of
 1,3-diethyl-2,2-dimethoxymethylcyclohexane as external electron
 donor in Ziegler-Natta catalysis)
 IT 432551-33-2P 432551-34-3P 432551-35-4P 432551-36-5P
 432551-37-6P 432551-38-7P 432551-39-8P
 (synthesis and evaluation of 1,3-diethyl-2,2-
 dimethoxymethylcyclohexane as external electron donor in
 Ziegler-Natta catalysis)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L63 ANSWER 4 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:499985 HCAPLUS¹
DOCUMENT NUMBER: 136:151503
TITLE: Synthesis and properties of N-vinyl-3-and
N-vinyl-5-pyrazolecarboxylic esters
AUTHOR(S): Attaryan, H. S.; Grigoryan, A. J.; Panossyan,
G. A.; Matsoyan, S. G.
CORPORATE SOURCE: Inst. Obshch. Neorg. Khim. im. M. G.
Manvelyan, NAN Respubl. Arm., Yerevan,
Armenia
SOURCE: Khimicheskii Zhurnal Armenii (2001), 54(1-2),
102-109
CODEN: KZARF3; ISSN: 1561-4190
PUBLISHER: Izdatel'stvo Gitutyun NAN Respubliki Armenii
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Esterification of pyrazolecarboxylic acid by aliphatic alcs. ROH
(R=CH₃, C₂H₅, iso-C₃H₇, C₄H₉) leads to the formation of
corresponding esters; vinylation of the esters in the presence of
mercury sulfate leads to the formation of N-vinyl-3- and
N-vinyl-5-pyrazolecarboxylic acids. **Polymerization** and
homopolymn. of the obtained monomers in the presence of a
radical initiator was studied. In both cases,
N-vinyl-5-pyrazolecarboxylic acid is more active. The reactivity
ratios in **polymerization** for Me esters were calculate r₁=0.71 and
r₂=2.7.
IT 1621-91-6, 3(5)-Pyrazolecarboxylic acid
(synthesis and **radical polymerization** of
N-vinyl-3- and N-vinyl-5-pyrazolecarboxylic esters)
RN 1621-91-6 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid (9CI) (CA INDEX NAME)

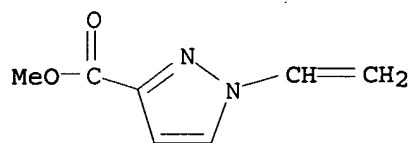


IT 69457-64-3P 122609-01-2P 122609-02-3P
122609-03-4P
(synthesis and **radical polymerization** of
N-vinyl-3- and N-vinyl-5-pyrazolecarboxylic esters)
RN 69457-64-3 HCAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-ethenyl-, ethyl ester (9CI) (CA
INDEX NAME)



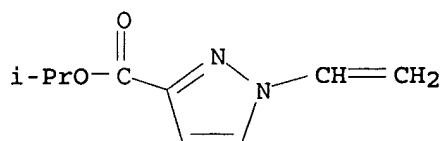
RN 122609-01-2 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 1-ethenyl-, methyl ester (9CI) (CA INDEX NAME)



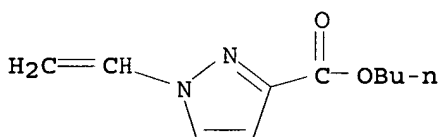
RN 122609-02-3 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 1-ethenyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 122609-03-4 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 1-ethenyl-, butyl ester (9CI) (CA INDEX NAME)



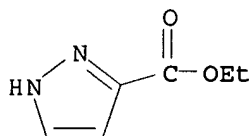
IT 5932-27-4, Ethyl 3-pyrazolecarboxylate 15366-34-4

122608-99-5 122609-00-1

(vinylation of esters of pyrazolecarboxylic acids)

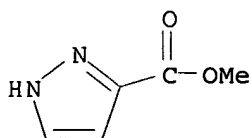
RN 5932-27-4 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, ethyl ester (9CI) (CA INDEX NAME)

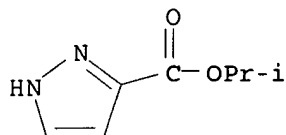


RN 15366-34-4 HCAPLUS

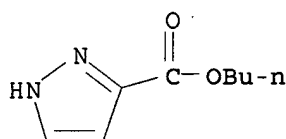
CN 1H-Pyrazole-3-carboxylic acid, methyl ester (9CI) (CA INDEX NAME)



RN 122608-99-5 HCAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, 1-methylethyl ester (9CI) (CA
 INDEX NAME)



RN 122609-00-1 HCAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, butyl ester (9CI) (CA INDEX NAME)



CC 35-4 (Chemistry of Synthetic High Polymers)
 ST vinyl pyrazolecarboxylic ester synthesis radical
 polymn copolymn
 IT Polymerization catalysts
 Reactivity ratio in polymerization
 (radical; synthesis and radical
 polymerization of N-vinyl-3- and N-vinyl-5-pyrazolecarboxylic
 esters)
 IT Hydrogen bond
 Vinylation catalysts
 (synthesis and radical polymerization of
 N-vinyl-3- and N-vinyl-5-pyrazolecarboxylic esters)
 IT 78-67-1, AIBN 7783-35-9, Mercury (II) sulfate
 (synthesis and radical polymerization of
 N-vinyl-3- and N-vinyl-5-pyrazolecarboxylic esters)
 IT 1621-91-6, 3(5)-Pyrazolecarboxylic acid
 (synthesis and radical polymerization of
 N-vinyl-3- and N-vinyl-5-pyrazolecarboxylic esters)
 IT 69457-64-3P 69457-66-5P 122609-01-2P
 122609-02-3P 122609-03-4P 122609-04-5P
 122609-05-6P 122818-18-2P
 (synthesis and radical polymerization of
 N-vinyl-3- and N-vinyl-5-pyrazolecarboxylic esters)
 IT 394658-30-1P
 (synthesis and radical polymerization of
 N-vinyl-3- and N-vinyl-5-pyrazolecarboxylic esters)
 IT 108-05-4, Vinyl acetate, reactions 5932-27-4, Ethyl
 3-pyrazolecarboxylate 5932-27-4 15366-34-4
 15366-34-4 122608-99-5 122608-99-5
 122609-00-1 122609-00-1
 (vinylation of esters of pyrazolecarboxylic acids)

L63 ANSWER 5 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2000:337094 HCAPLUS
 DOCUMENT NUMBER: 133:74062
 TITLE: Macrocyclization of α -(alkynyloxy)silyl-
 α -diazoacetates by inter-/intramolecular

[3+2] cycloaddition reaction sequences

AUTHOR(S): Maas, Gerhard; Gettwert, Volker; Krebs, Fred; Schmidtberg, Gunter

CORPORATE SOURCE: Abteilung Organische Chemie I. Universitat Ulm, Ulm, 89081, Germany

SOURCE: Chemistry--A European Journal (2000), 6(9), 1646-1655

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

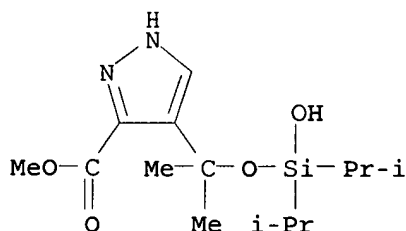
LANGUAGE: English

AB Thermally induced intra-/intermol. [3+2] cycloaddn. reaction sequences of α -(alkynyloxy)silyl- α -diazoacetates 1 lead to [3.3](1,4)pyrazolophanes (2)2 and higher cyclooligomers thereof [(2)n, n > 2]. In most cases, the cyclodimer was isolated by crystallization, while a complete separation of the mixture of the higher cyclooligomers was not possible. Solid state structures of cyclodimers (2b)2 and (2c)2, cyclotrimer (2b)3, and cyclotetramer (2e)4 were determined by x-ray diffraction anal. Field-desorption mass spectra were used to characterize the cyclooligomer mixts. The relative amts. of the cyclooligomers depend on the substitution pattern of the diazo compound. The cyclooligomerization reactions reported herein demonstrate, for the 1st time, the involvement of diazo functions in macrocyclization reactions via 1,3-dipolar cycloaddn.

IT 279694-31-4P 279694-33-6P
(preparation and fluoride-induced desilylation reaction of)

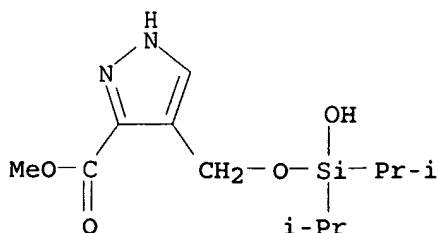
RN 279694-31-4 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-[1-[[hydroxybis(1-methylethyl)silyl]oxy]-1-methylethyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 279694-33-6 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-[[[hydroxybis(1-methylethyl)silyl]oxy]methyl]-, methyl ester (9CI) (CA INDEX NAME)

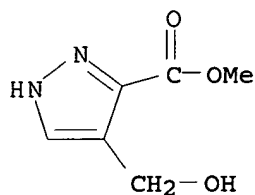


IT 124598-39-6P 279694-34-7P 279694-35-8P

279694-36-9P

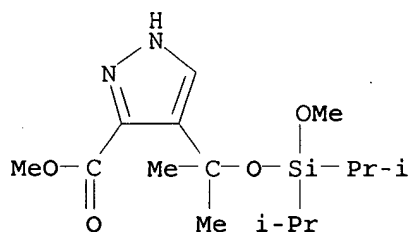
(preparation of)

RN 124598-39-6 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-(hydroxymethyl)-, methyl ester
(9CI) (CA INDEX NAME)

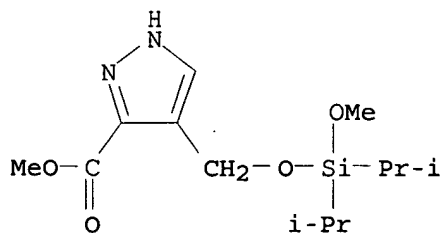
RN 279694-34-7 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-[1-[[methoxybis(1-methylethyl)silyl]oxy]-1-methylethyl]-, methyl ester (9CI) (CA INDEX NAME)



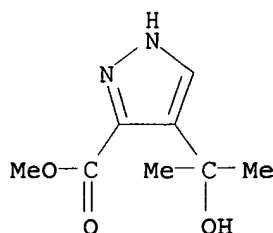
RN 279694-35-8 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-[[[methoxybis(1-methylethyl)silyl]oxy]methyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 279694-36-9 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-(1-hydroxy-1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 35, 75

IT **Polymerization**

(cyclooligomerization; of α -(alkynyloxy)silyl- α -
diazoacetates by inter-/intramol. [3+2] cycloaddn. reaction
sequences)

IT 279694-31-4P 279694-33-6P

(preparation and fluoride-induced desilylation reaction of)

IT 124598-39-6P 279694-22-3P 279694-32-5P

279694-34-7P 279694-35-8P 279694-36-9P

(preparation of)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L63 ANSWER 6 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:208120 HCAPLUS

DOCUMENT NUMBER: 132:334949

TITLE: Aromatic benzobisazole polymers based on
1H-pyrazole-3,5-diyl moiety

AUTHOR(S): Dang, T. D.; Venkatasubramanian, N.; Arnold,
F. E.

CORPORATE SOURCE: AFRL/MLBP, Materials and Manufacturing
Technology Directorate, Dayton, OH,
45433-7750, USA

SOURCE: Polymer Preprints (American Chemical Society,
Division of Polymer Chemistry) (2000), 41(1),
217-218

CODEN: ACPPAY; ISSN: 0032-3934

PUBLISHER: American Chemical Society, Division of Polymer
Chemistry

DOCUMENT TYPE: Journal

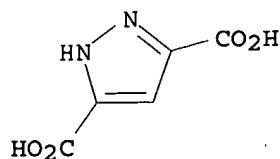
LANGUAGE: English

AB Aromatic benzobisazole polymers containing the heteroarom.
1H-pyrazole-3,5-diyl moiety were synthesized in moderate to high
mol. wts., as indicated by intrinsic viscosities, from
1H-pyrazole-3,5-dicarboxylic acid or the corresponding diacid
chloride. The lyotropic liquid crystalline behavior of the benzobisazole
system was demonstrated in the case of poly(benzobisoxazole) in
polyphosphoric acid, via the observation of optical birefringence.

IT 3112-31-0, 3,5-Pyrazoledicarboxylic acid
(in preparation and property of aromatic benzobisazole polymers based
on 1H-pyrazole-3,5-diyl moiety)

RN 3112-31-0 HCAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid (9CI) (CA INDEX NAME)



CC 35-5 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 75

IT Liquid crystals, **polymeric**

(lyotropic; preparation and property of aromatic benzobisazole polymers based on 1H-pyrazole-3,5-diyl moiety)

IT 95-55-6, 2-Aminophenol 137-07-5, 2-Aminothiophenol

3112-31-0, 3,5-Pyrazoledicarboxylic acid

(in preparation and property of aromatic benzobisazole polymers based on 1H-pyrazole-3,5-diyl moiety)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L63 ANSWER 7 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:164794 HCAPLUS

DOCUMENT NUMBER: 132:279564

TITLE: Synthesis and reactivity of dialkyl
1-vinylpyrazole-3,5-dicarboxylates in
radical polymerization

AUTHOR(S): Shatalov, G. V.; Preobrazhenskii, S. A.;
Kuznetsov, V. A.

CORPORATE SOURCE: Russia

SOURCE: Izvestiya Vysshikh Uchebnykh Zavedenii,
Khimiya i Khimicheskaya Tekhnologiya (1999),
42(5), 62-64

CODEN: IVUKAR; ISSN: 0579-2991

PUBLISHER: Ivanovskii Gosudarstvennyi
Khimiko-Tekhnologicheskii Universitet

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The derivs. of pyrazole-3,5-dicarboxylic acid dialkyl esters have been prepared The kinetics of their **radical polymerization** in dioxane and copolymn. with Me methacrylate have been studied. The dependence has been found between the **polymerization** rate and the number of C atoms in aliphatic chain of ester components and that in a pyrazole cycle. The Alfrey-Price consts. and copolymn. parameters were determined

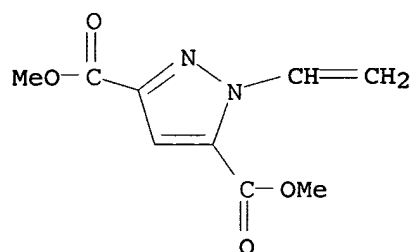
IT 86797-83-3P 263875-81-6P 263875-82-7P

263875-83-8P 263875-84-9P

(preparation and **polymerization**; preparation and reactivity of dialkyl vinylpyrazoledicarboxylates in **radical polymn**
)

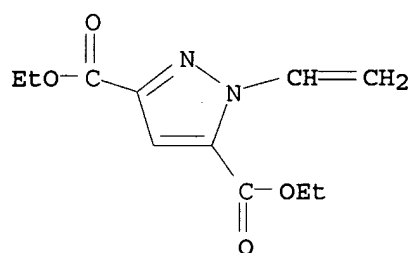
RN 86797-83-3 HCAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid, 1-ethenyl-, dimethyl ester
(9CI) (CA INDEX NAME)



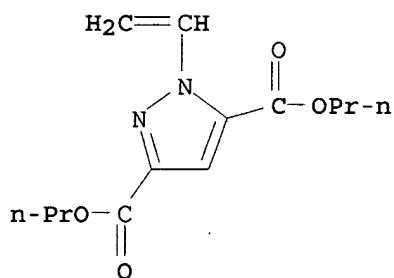
RN 263875-81-6 HCAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid, 1-ethenyl-, diethyl ester (9CI)
(CA INDEX NAME)



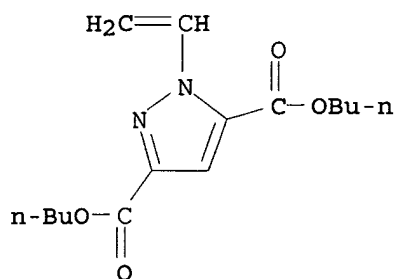
RN 263875-82-7 HCAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid, 1-ethenyl-, dipropyl ester
(9CI) (CA INDEX NAME)

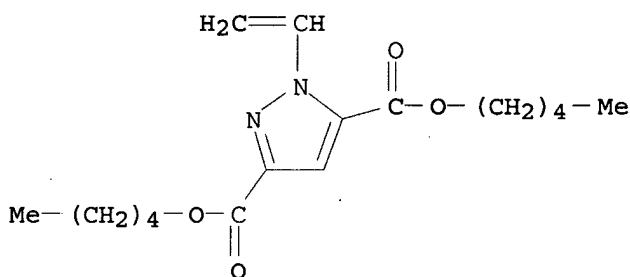


RN 263875-83-8 HCAPLUS

CN 1H-Pyrazole-3,5-dicarboxylic acid, 1-ethenyl-, dibutyl ester (9CI)
(CA INDEX NAME)



RN 263875-84-9 HCAPLUS
 CN 1H-Pyrazole-3,5-dicarboxylic acid, 1-ethenyl-, dipentyl ester
 (9CI) (CA INDEX NAME)

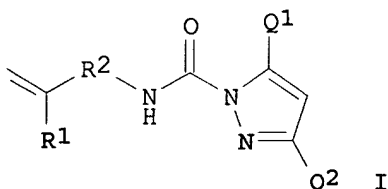


CC 35-2 (Chemistry of Synthetic High Polymers)
 ST vinylpyrazoledicarboxylate ester prepn monomer;
 vinylpyrazoledicarboxylic acid ester **radical**
polymn kinetics; polyvinylpyrazoledicarboxylate ester
 prepn **radical polymn**; methyl methacrylate
radical copolymn vinylpyrazoledicarboxylate ester
 IT Q-e value in **polymerization**
 (preparation and reactivity of dialkyl vinylpyrazoledicarboxylates
 in **radical polymerization**)
 IT **Polymerization**
 (radical; preparation and reactivity of dialkyl
 vinylpyrazoledicarboxylates in)
 IT **Polymerization** kinetics
 (radical; preparation and reactivity of dialkyl
 vinylpyrazoledicarboxylates in **radical polymn**
 .)
 IT 86797-83-3P 263875-81-6P 263875-82-7P
 263875-83-8P 263875-84-9P
 (preparation and **polymerization**; preparation and reactivity of dialkyl
 vinylpyrazoledicarboxylates in **radical polymn**
 .)
 IT 86797-84-4P 263875-85-0P 263875-86-1P 263875-87-2P
 263875-88-3P, Methyl methacrylate-1-vinylpyrazole-3,5-dicarboxylic
 acid dimethyl ester copolymer 263875-89-4P, Methyl
 methacrylate-1-vinylpyrazole-3,5-dicarboxylic acid diethyl ester
 copolymer 263875-90-7P, Methyl methacrylate-1-vinylpyrazole-3,5-
 dicarboxylic acid dipropyl ester copolymer 263875-91-8P, Methyl
 methacrylate-1-vinylpyrazole-3,5-dicarboxylic acid dibutyl ester
 copolymer
 (preparation and reactivity of dialkyl vinylpyrazoledicarboxylates

in radical polymerization)

L63 ANSWER 8 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1998:768080 HCAPLUS
 DOCUMENT NUMBER: 130:53771
 TITLE: Pyrazoles and their compositions curable at low temperature having excellent storage stability
 INVENTOR(S): Matsuhira, Shinya; Misu, Tadanao; Futagami, Masato; Hatanaka, Masashi; Kihara, Muneyo
 PATENT ASSIGNEE(S): Showa Denko K. K., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

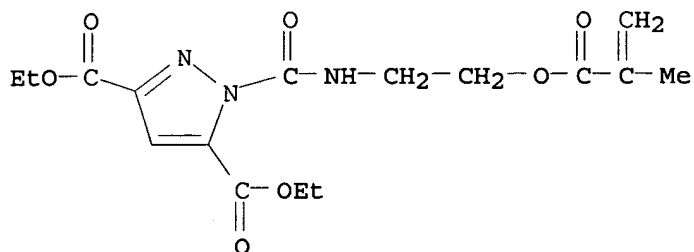
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10316663	A2	19981202	JP 1997-128289	1997 0519
JP 2006104215	A2	20060420	JP 2005-366456	2005 1220
PRIORITY APPLN. INFO.:			JP 1997-128289	A3 1997 0519
OTHER SOURCE(S):		MARPAT 130:53771		



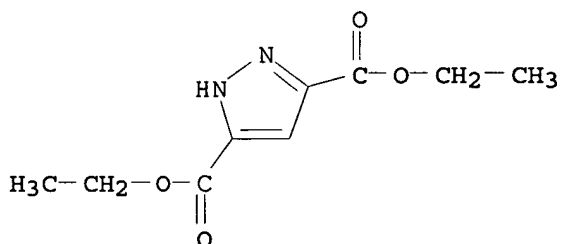
AB Title compds. are I (R1, R4, R5 = H, Me; R2 = CO, CO2R3, C6H4CR4R5, CO2CH2CH2O2CNHR6; R3 = C2-6 alkylene; R6 = divalent diisocyanate residue; Q1, Q2 = H, Me, RCONH, ROCO; R = alkyl). The compns., useful for coatings and adhesives with good appearance and hardness, comprise (a) copolymers containing I and unsatd. compds. OH, H2N, or CO2H group as monomer components or (b) copolymers containing I as monomer components and polymers containing OH, H2N, or CO2H group. Thus, 20 g compound prepared from 3,5-dimethylpyrazole and Karenzu MOI (2-methacryloyloxyethyl isocyanate), 8 g styrene, 20 g Me methacrylate, 40 g Bu acrylate, and 10 g hydroxyethyl methacrylate were polymerized in cyclohexanone at 70° for 4 h in the presence of 2,2'-azobis(4-methoxy-2,4-dimethylvaleronitrile) to give a

copolymer solution, which was applied on a glass plate to give a film showing good peeling resistance.

- IT 217437-48-4P
(pyrazoles and their compns. curable at low temperature having excellent storage stability)
- RN 217437-48-4 HCAPLUS
- CN 1H-Pyrazole-3,5-dicarboxylic acid, 1-[[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]amino]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)



- IT 37687-24-4, Pyrazole-3,5-dicarboxylic acid diethyl ester
(pyrazoles and their compns. curable at low temperature having excellent storage stability)
- RN 37687-24-4 HCAPLUS
- CN 1H-Pyrazole-3,5-dicarboxylic acid, diethyl ester (9CI) (CA INDEX NAME)



- IC ICM C07D231-12
ICS C07D231-14; C08F212-02; C08F220-36; C08F220-60; C08F290-00; C08F299-00
- CC 42-10 (Coatings, Inks, and Related Products)
Section cross-reference(s): 35
- IT 67-51-6DP, 3,5-Dimethylpyrazole, reaction products with trimethylisocyanatomethylcyclohexyl isocyanate and hydroxyethyl methacrylate 868-77-9DP, 2-Hydroxyethyl methacrylate, reaction products with trimethylisocyanatomethylcyclohexyl isocyanate and dimethylpyrazole 4098-71-9DP, reaction products with hydroxyethyl methacrylate and dimethylpyrazole 217437-46-2P 217437-47-3P 217437-48-4P
(pyrazoles and their compns. curable at low temperature having excellent storage stability)
- IT 67-51-6, 3,5-Dimethylpyrazole 2094-99-7 4474-60-6, Methacryloyl isocyanate 30674-80-7 37687-24-4, Pyrazole-3,5-dicarboxylic acid diethyl ester
(pyrazoles and their compns. curable at low temperature having excellent storage stability)

L63 ANSWER 9 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1998:479597 HCAPLUS
 DOCUMENT NUMBER: 129:110446
 TITLE: Compositions containing perfume incorporated
 in polymer particles
 INVENTOR(S): Ness, Jeremy Nicholas; Irving, Pamela
 Virginia; Goodall, Marcus James
 PATENT ASSIGNEE(S): Quest International B.V., Neth.
 SOURCE: PCT Int. Appl., 77 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9828396	A1	19980702	WO 1997-GB3529	1997 1223
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W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2275792	AA	19980702	CA 1997-2275792	1997 1223
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AU 9853317	A1	19980717	AU 1998-53317	1997 1223
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AU 729041	B2	20010125		
ZA 9711578	A	19990623	ZA 1997-11578	1997 1223
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ZA 9711582	A	19990623	ZA 1997-11582	1997 1223
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ZA 9711589	A	19990623	ZA 1997-11589	1997 1223
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EP 950087	A1	19991020	EP 1997-950315	1997 1223
<--				
R: DE, ES, FR, GB, IT, NL				
US 6024943	A	20000215	US 1997-997380	1997

1223

BR 9713634 A 20000411 BR 1997-13634

1997
1223

US 6194375 B1 20010227 US 1997-996721

1997
1223

JP 2001507058 T2 20010529 JP 1998-528553

1997
1223

PT 950070 T 20020628 PT 1997-950317

1997
1223

ES 2170969 T3 20020816 ES 1997-950317

1997
1223

PRIORITY APPLN. INFO.: EP 1996-309466 A

1996
1223

WO 1997-GB3529 W

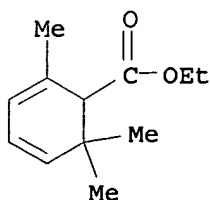
1997
1223

AB Perfume is absorbed within organic polymer particles which have a further polymer at their exterior. The further polymer incorporates free OH groups and serves to promote deposition of the particles from a wash or rinse liquor. The further polymer may be part of an encapsulating shell, but more conveniently is used as a stabilizer during polymerization of the particles. Highly hydrolyzed poly(vinyl alc.) (PVA) is preferred. For example, 1,6-hexanediol diacrylate-styrene copolymer beads were prepared by radical dispersion polymerization in the presence of PVA (Gohsenol AH-22), a mixture of perfumes and di(hardened tallow)dimethylammonium chloride was stirred with the beads in H₂O, and the beads combined with a rinse conditioner to show good retention of perfume in cotton terry toweling fabrics treated with the conditioner.

IT 35044-57-6
(perfume; compns. containing perfume incorporated in polymer particles)

RN 35044-57-6 HCAPLUS

CN 2,4-Cyclohexadiene-1-carboxylic acid, 2,6,6-trimethyl-, ethyl ester (9CI) (CA INDEX NAME)



IC ICM C11D003-50
ICS C11D017-00; C11D017-04
CC 46-5 (Surface Active Agents and Detergents)
Section cross-reference(s): 38
IT 60-12-8, Phenylethyl alcohol 66-25-1, Hexanal 78-70-6
80-54-6, Lilial 91-64-5, Coumarin 97-53-0, Eugenol 104-67-6,
 γ -Undecalactone 106-22-9, Citronellol 115-95-7, Linalyl
acetate 118-58-1, Benzyl salicylate 120-57-0, Heliotropin
151-05-3, Dimethylbenzylcarbonyl acetate 2437-25-4,
Dodecanenitrile 2630-39-9, Methyl dihydrojasmonate 5989-27-5
6259-76-3, Hexyl salicylate 6485-40-1, L-Carvone 21145-77-7,
Tonalid 25265-71-8, Dipropylene glycol 30385-25-2,
Dihydromyrcenol 32210-23-4, p-tert-Butylcyclohexyl acetate
35044-57-6 39350-49-7, Hexylcinnamic aldehyde
43052-87-5, α -Damascone 50984-52-6, Anisaldehyde
56011-02-0, Anther 65405-77-8, cis-3-Hexenyl salicylate
67874-81-1, Cedramber 106354-02-3 124899-75-8 210035-91-9
210035-92-0
(perfume; compns. containing perfume incorporated in polymer
particles)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L63 ANSWER 10 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:127204 HCAPLUS

DOCUMENT NUMBER: 126:118281

TITLE: Soluble and Colorless Polyimides from
Bicyclo[2.2.2]octane-2,3,5,6-tetracarboxylic
2,3:5,6-Dianhydrides

AUTHOR(S): Matsumoto, Toshihiko; Kurosaki, Toshikazu

CORPORATE SOURCE: Department of Industrial Chemistry Faculty of
Engineering, Tokyo Institute of Polytechnics,
Kanagawa, 243-02, Japan

SOURCE: Macromolecules (1997), 30(4), 993-1000

CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

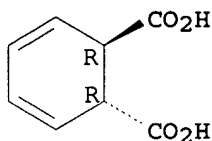
LANGUAGE: English

AB Two tetracarboxylic dianhydrides with a polyalicyclic structure,
bicyclo[2.2.2]octane-2-endo,3-endo,5-exo,6-exo-tetracarboxylic
2,3:5,6-dianhydride (I) and bicyclo[2.2.2]octane-2-exo,3-exo,5-
exo,6-exo-tetracarboxylic 2,3:5,6-dianhydride, were synthesized,
and polycondensations of the dianhydrides with aromatic diamines were
carried out in well-purified N,N-dimethylacetamide (DMAC) at
85°-105° under N. The resulting poly(amic acid)s as
precipitated possessed inherent viscosities in the range 0.5-0.1 dL/g.
Some of the poly(amic acid)s formed flexible and tough films after
curing. Polyimides were also obtained by a thermal solution
imidization method where the DMAC solns. of poly(amic acid)s were
heated at reflux temperature for 6 h. All of the examined polyimides were
soluble at room temperature in aprotic and protic polar solvents such as
DMAC and m-cresol. All of the polyimides showed excellent thermal
stability with no significant weight loss up to approx. 400°,
and the 5% weight loss temps. in N were over 450°. The
polyimides had glass transition temps. over 380° except for
the polyimides using 1,3-bis(4-aminophenoxy)benzene as an aromatic
diamine. The flexible polyimide films possessed a tensile modulus
range of 1.5-2.6 GPa, a tensile strength range of 52-96 MPa, an

elongation at break of 3-11%, and a dielec. constant range of 3.2-3.7. These films exhibited cutoffs at wavelengths shorter than 320 nm and were entirely colorless. Normalized transparencies in the visible region (400-780 nm) were over 86% and, notably, the film prepared from I and 4,4'-diaminodiphenyl ether had an excellent transparency of 94%. Colorlessness and transparency of the film at room temperature were maintained up to 200° when the film was heated in air and to 400° in N. The polyimide of which the end group (the aromatic amino group) was capped using acetic anhydride was almost colorless even when heated at 300° in air.

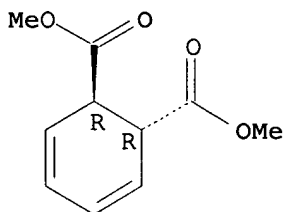
IT 5675-13-8P 26549-64-4P
 (intermediate; in preparation of soluble and colorless polyimides from bicyclo[2.2.2]octane-2,3,5,6-tetracarboxylic 2,3:5,6-dianhydrides and aromatic diamines)
 RN 5675-13-8 HCAPLUS
 CN 3,5-Cyclohexadiene-1,2-dicarboxylic acid, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 26549-64-4 HCAPLUS
 CN 3,5-Cyclohexadiene-1,2-dicarboxylic acid, dimethyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 35-5 (Chemistry of Synthetic High Polymers)
 IT Polymerization
 (of bicyclo[2.2.2]octane-2,3,5,6-tetracarboxylic 2,3:5,6-dianhydrides with aromatic diamines)
 IT 5675-13-8P 26549-64-4P 56782-33-3P
 108211-23-0P
 (intermediate; in preparation of soluble and colorless polyimides from bicyclo[2.2.2]octane-2,3,5,6-tetracarboxylic 2,3:5,6-dianhydrides and aromatic diamines)

L63 ANSWER 11 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1997:120743 HCAPLUS
 DOCUMENT NUMBER: 126:211739
 TITLE: Reaction of sulfuric anhydride with cyclohexane
 AUTHOR(S): Makitra, R. G.

CORPORATE SOURCE: Inst. Fiz. Khim., Nats. Akad. Nauk Ukr., Lvov, Ukraine

SOURCE: Zhurnal Obshchei Khimii (1996), 66(10), 1710-1714
CODEN: ZOKHAA4; ISSN: 0044-460X

PUBLISHER: Nauka

DOCUMENT TYPE: Journal

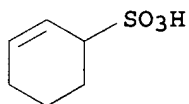
LANGUAGE: Russian

AB The products of sulfation of cyclohexane with SO₃(g) followed by hydrolysis were separated by extraction with isoamyl alc. and found to be identical to those formed in oleum: in the aqueous layer remained hydroxy di- and polysulfonic acids that themselves were separated as two groups of salts of varying solubility in 75% alc. The first group (I) consisted of hydroxy di- and trisulfonic acids that were soluble in 6 N H₂SO₄ (and from which they could not be extracted with isoamyl alc.) whose K salts were soluble in 75% alc.; the K salt of the second group (II) was insol. in 75% alc. and consisted of polyhydroxy polysulfonic acids or **polymeric** sulfonic acids. The alc. extract was subsequently dissolved in 6 N H₂SO₄, extracted with isoamyl alc., and neutralized with KOH to afforded K 2-cyclohexenesulfonate. The anal. methods of E. Gerhards and W. Dirscherle (1961) who claimed to isolate a single product with anticoagulant activity in the SO₃(g) reaction were challenged in the present paper.

IT 188046-94-8P, 2-Cyclohexene-1-sulfonic acid
(sulfonation of cyclohexane with sulfuric anhydride and oleum)

RN 188046-94-8 HCAPLUS

CN 2-Cyclohexene-1-sulfonic acid (9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 1, 35

IT 188046-94-8P, 2-Cyclohexene-1-sulfonic acid 188046-95-9P
188046-96-0P
(sulfonation of cyclohexane with sulfuric anhydride and oleum)

L63 ANSWER 12 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:379869 HCAPLUS

DOCUMENT NUMBER: 125:34355

TITLE: Metal complexes containing non-aromatic, anionic, dienyl groups and addition **polymerization** catalysts therefrom

INVENTOR(S): Wilson, David R.; Neithamer, David R.; Nickias, Peter N.; Kruper, W. Jack, Jr.

PATENT ASSIGNEE(S): Dow Chemical Company, USA

SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2

DOCUMENT TYPE: **Patent**

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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 WO 9608498 A1 19960321 WO 1995-US8489
1995
0706

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W: CA, JP
 RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL,
 PT, SE
 US 5541349 A 19960730 US 1994-304301
1994
0912

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CA 2196893 AA 19960321 CA 1995-2196893
1995
0706

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EP 781288 A1 19970702 EP 1995-926187
1995
0706

<--

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC,
 NL, PT, SE
 JP 10507163 T2 19980714 JP 1995-510169
1995
0706

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PRIORITY APPLN. INFO.: US 1994-304301 A
1994
0912

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WO 1995-US8489 W
1995
0706

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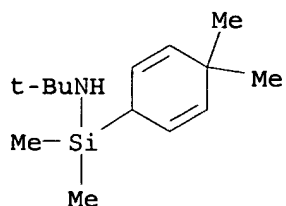
OTHER SOURCE(S): MARPAT 125:34355

AB Catalytic derivs. of group 4 metal complexes wherein the metal is
 in the +2 or +4 formal oxidation state containing a cyclic or noncyclic,
 non-aromatic, anionic, dienyl ligand group bound to the metal and
 having a bridged ligand structure [e.g., (N-tert-
 butylamido) (dimethyl) (6,6-dimethyl- η 5-cyclohexadien-3-
 yl)silane titanium(IV) dichloride] including novel zwitterionic
 complexes are useful for **polymerizing** addition
polymerizable monomers (e.g., ethylene and 1-octene).

IT 176162-74-6P
 (metal complexes containing non-aromatic, anionic, dienyl groups for
 addition **polymerization** catalysts)

RN 176162-74-6 HCAPLUS

CN Silanamine, 1-(4,4-dimethyl-2,5-cyclohexadien-1-yl)-N-(1,1-
 dimethylethyl)-1,1-dimethyl- (9CI) (CA INDEX NAME)



IC ICM C07F007-00
ICS C07F007-10; C08F010-00

CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67

ST **polymn** catalyst ethylene octene copolymer; metal complex
addn **polymn** catalyst; cyclohexadiene deriv addn
polymn catalyst; cyclopentadiene deriv addn **polymn**
catalyst; silane complex addn **polymn** catalyst

IT **Polymerization** catalysts
(metal complexes containing non-aromatic, anionic, dienyl groups for
addition **polymerization** catalysts)

IT Chlorides, preparation
Zwitterionic compounds
(**polymerization** catalysts; metal complexes containing non-aromatic,
anionic, dienyl groups for addition **polymerization** catalysts)

IT 176162-85-9P 177717-14-5P 177991-15-0P 177991-16-1P
177991-17-2P 177991-18-3P 177991-19-4P 177991-20-7P
177991-21-8P 177991-22-9P 177991-23-0P 177991-24-1P
(addition **polymerization** catalysts; metal complexes containing
non-aromatic, anionic, dienyl groups for addition **polymerization**
catalysts)

IT 26221-73-8P, Ethylene-1-octene copolymer
(catalysts for; metal complexes containing non-aromatic, anionic,
dienyl groups for addition **polymerization** catalysts)

IT 33482-80-3P, 5,5-Dimethyl-1,3-cyclohexadiene 35934-83-9P,
3,3-Dimethyl-1,4-cyclohexadiene 82360-21-2P 176162-74-6P
176162-75-7P
(metal complexes containing non-aromatic, anionic, dienyl groups for
addition **polymerization** catalysts)

IT 109-72-8, n-Butyl lithium, reactions 126-81-8,
5,5-Dimethyl-1,3-cyclohexanedione 7550-45-0, Titanium
tetrachloride, reactions 10026-11-6, Zirconium tetrachloride
41233-93-6
(metal complexes containing non-aromatic, anionic, dienyl groups for
addition **polymerization** catalysts)

L63 ANSWER 13 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:191626 HCAPLUS

DOCUMENT NUMBER: 124:262041

TITLE: Heat-resistant stereoregular polyimides
prepared from bicyclo[2.2.2]octane-2,3,5,6-
tetracarboxylic dianhydrides

INVENTOR(S): Matsumoto, Toshihiko; Kurosaki, Juichi; Oono,
Toshinobu; Nishiguchi, Ikuzo

PATENT ASSIGNEE(S): Maruzen Oil Co Ltd, Japan; Osaka City

SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 07304868	A2	19951121	JP 1994-119610	1994 0509

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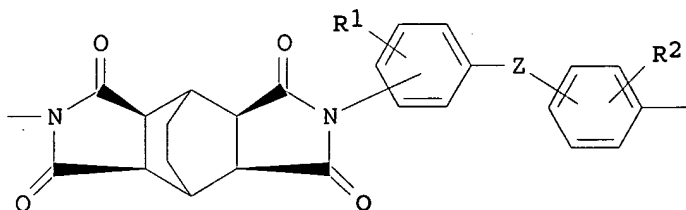
PRIORITY APPLN. INFO.:

JP 1994-119610

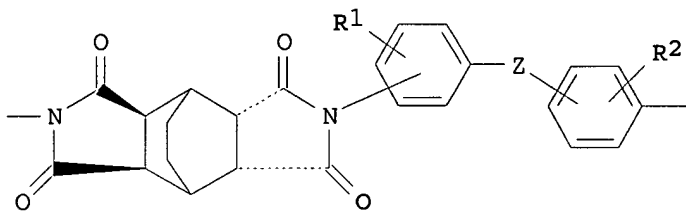
1994
0509

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I



II

AB The title polyimides with units I or II (R_1 , R_2 = H, halo, Me, etc.; Z = linking group) are prepared. The polyimides are soluble in organic solvents and useful for elec. insulating membranes for semiconductors, orientation films for liquid crystals, etc.

Polymerizing 4,4'-diaminodiphenyl ether with 1rC7-bicyclo[2.2.2]octane-2t,3t,5c,6c-tetracarboxylic 2,3:5,6-dianhydride and in N-methyl-2-pyrrolidone gave a polyimide which was soluble in DMF, pyridine, DMSO, etc.

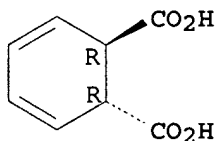
IT 5675-13-8 26549-64-4

(in preparation of stereoregular bicyclooctanetetracarboxylic dianhydride)

RN 5675-13-8 HCAPLUS

CN 3,5-Cyclohexadiene-1,2-dicarboxylic acid, (1R,2R)-rel- (9CI) (CA INDEX NAME)

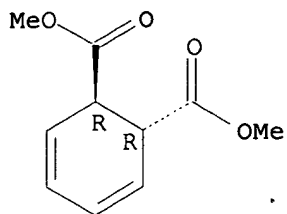
Relative stereochemistry.



RN 26549-64-4 HCAPLUS

CN 3,5-Cyclohexadiene-1,2-dicarboxylic acid, dimethyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



(1) d. 5,6

IC ICM C08G073-10
 CC 35-5 (Chemistry of Synthetic High Polymers)
 Section cross-reference(s): 37
 IT 624-48-6, Dimethyl maleate 5675-13-8 26549-64-4
 (in preparation of stereoregular bicyclooctanetetracarboxylic dianhydride)
 IT 175275-19-1P 175275-20-4P
 (preparation and **polymerization** with aromatic diamines to give polyimides)

L63 ANSWER 14 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:191607 HCAPLUS

DOCUMENT NUMBER: 124:318144

TITLE: Metal (III) complexes containing conjugated, nonaromatic anionic II-bound groups and addition **polymerization** catalysts from them

INVENTOR(S): Wilson, David R.; Neithamer, David R.; Nickias, Peter N.; Kruper, W. Jack, Jr.

PATENT ASSIGNEE(S): The Dow Chemical Company, USA

SOURCE: U.S., 16 pp.

CODEN: USXXAM

DOCUMENT TYPE: **Patent**
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5495036	A	19960227	US 1994-304315	1994 0912
CA 2196896	AA	19960321	CA 1995-2196896	1995 0706
WO 9608497	A1	19960321	WO 1995-US8466	1995 0706
EP 781287	A1	19970702	EP 1995-925522	1995 0706

W: CA, JP
 RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL,
 PT, SE

EP 781287 B1 20020102
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC,
 NL, PT, SE
 JP 10505609 T2 19980602 JP 1996-510167

1995
 0706

AT 211478 E 20020115 AT 1995-925522

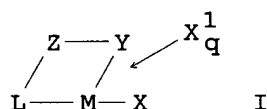
1995
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PRIORITY APPLN. INFO.:

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 US 1994-304315 A
 1994
 0912

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 WO 1995-US8466 W
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 0706

OTHER SOURCE(S): MARPAT 124:318144
 GI



AB Title complexes I [M is a Group 3, Group 4, or lanthanide metal in the +3 formal oxidation state; L is a (cyclic) nonarom. anionic, dienyl ligand group containing ≤ 60 nonhydrogen atoms; Z = B or Group 14 element moiety containing ≤ 60 nonhydrogen atoms; Y = N-, P-, S-, or O-containing group having ≤ 20 nonhydrogen atoms; X = monovalent anionic moiety containing ≤ 20 nonhydrogen atoms, not an aromatic group π -bonded to M; X' = a Lewis base containing ≤ 40 nonhydrogen atoms; X and X' may be bonded together forming a moiety that is both covalently bound to M and coordinated thereto via Lewis base functionality; q = 0-3] are prepared and used in addition **polymerization**, alone or with a cocatalyst, to give degradation-resistant polymers due to less unsatn. Thus, (N-tert-butylamido) (dimethyl) (6,6-dimethyl- η 5-cyclohexadien-3-yl)silanetitanium(III) 2-(dimethylamino)benzyl was prepared and used with ferrocenium tetrakis(pentafluorophenyl)borate to **polymerize** ethylene with 1-octene.

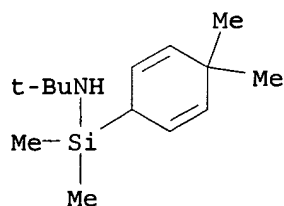
IT 176162-74-6P

(preparation and reaction in preparation of; metal (III) complexes containing

conjugated, nonarom. anionic II-bound groups and addition **polymerization** catalysts from them)

RN 176162-74-6 HCAPLUS

CN Silanamine, 1-(4,4-dimethyl-2,5-cyclohexadien-1-yl)-N-(1,1-dimethylethyl)-1,1-dimethyl- (9CI) (CA INDEX NAME)



IC ICM C07F007-28
 INCL 556012000
 CC 35-3 (Chemistry of Synthetic High Polymers)
 ST metal complex catalyst prepn addn **polymn**; lanthanide complex **polymn** catalyst prepn; rare earth metal complex catalyst prepn; coordination metal complex **polymn** catalyst prepn; ethylene octene copolymn metal complex catalyst; titanium complex catalyst prepn addn **polymn**
 IT **Polymerization catalysts**
 (metal (III) complexes containing conjugated, nonarom. anionic II-bound groups and addition **polymerization** catalysts from them)
 IT Rare earth metals, preparation
 (metal (III) complexes containing conjugated, nonarom. anionic II-bound groups and addition **polymerization** catalysts from them)
 IT Aluminoxanes
 (Me, cocatalyst; with metal (III) complexes containing conjugated, nonarom. anionic II-bound groups in addition **polymerization** of ethylene and octene)
 IT Alkenes, preparation
 (polymers, metal (III) complexes containing conjugated, nonarom. anionic II-bound groups and addition **polymerization** catalysts from them)
 IT 176162-77-9 176162-86-0 176162-87-1 176162-88-2
 176162-89-3 176162-90-6 176162-91-7 176162-92-8
 176162-93-9 176162-94-0 176162-95-1 176162-96-2
 176162-97-3 176162-98-4 176162-99-5 176163-00-1
 176163-01-2 176163-02-3 176163-03-4 176163-04-5
 176163-05-6 176163-06-7 176163-07-8 176163-08-9
 176163-09-0
 (catalyst; metal (III) complexes containing conjugated, nonarom. anionic II-bound groups and addition **polymerization** catalysts from them)
 IT 176162-79-1P 176162-80-4P 176162-84-8P
 (catalyst; metal (III) complexes containing conjugated, nonarom. anionic II-bound groups and addition **polymerization** catalysts from them)
 IT 135348-57-1
 (cocatalyst; with metal (III) complexes containing conjugated, nonarom. anionic II-bound groups in addition **polymerization** of ethylene and octene)
 IT 26221-73-8P
 (metal (III) complexes containing conjugated, nonarom. anionic II-bound groups and addition **polymerization** catalysts from them)
 IT 10060-17-0P, Diphenylmethyl potassium 33482-80-3P,
 5,5-Dimethyl-1,3-cyclohexadiene 35934-83-9P,
 3,3-Dimethyl-1,4-cyclohexadiene 82360-21-2P 176162-74-6P
 176162-75-7P 176162-76-8P 176162-78-0P 176162-81-5P

176162-82-6P 176162-83-7P 176162-85-9P 176329-27-4P
176329-29-6P

(preparation and reaction in preparation of; metal (III) complexes containing

conjugated, nonarom. anionic II-bound groups and addition
polymerization catalysts from them)

IT 41233-93-6P

(reaction in preparation of; metal (III) complexes containing
conjugated, nonarom. anionic II-bound groups and addition
polymerization catalysts from them)

IT 101-81-5, Diphenylmethane 109-72-8, n-Butyllithium, reactions

2733-79-1 18039-90-2 60556-33-4 64308-58-3 153813-71-9

(reaction in preparation of; metal (III) complexes containing
conjugated, nonarom. anionic II-bound groups and addition
polymerization catalysts from them)

IT 16853-85-3, Lithium aluminum hydride

(reduction by; metal (III) complexes containing conjugated, nonarom.
anionic II-bound groups and addition **polymerization** catalysts
from them)

IT 126-81-8, 5,5-Dimethyl-1,3-cyclohexanedione

(reduction in manufacture of; metal (III) complexes containing conjugated,
nonarom. anionic II-bound groups and addition **polymerization**
catalysts from them)

L63 ANSWER 15 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:636445 HCAPLUS

DOCUMENT NUMBER: 123:287156

TITLE: Preparation of propene block copolymers with
high impact resistance and rigidity

INVENTOR(S): Nomura, Yasuo; Taki, Noryuki; Nakajima,
Masashi; Ueki, Satoshi; Ishihara, Takeshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 07097411	A2	19950411	JP 1993-241628	1993 0928

PRIORITY APPLN. INFO.: <--
JP 1993-241628

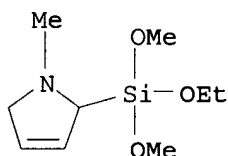
1993
0928

OTHER SOURCE(S): MARPAT 123:287156

AB The title copolymers are prepared by **polymerizing** propene to
give crystalline polypropene and subsequently copolymerizing propene and
ethylene in the presence of catalyst components obtained by
contacting solid catalyst components containing metal oxides, Mg, Ti,
halogen, and electron donors with olefins in the presence of organic
Al compds. and silanes $R_1xSiR_2y(OR_3)z$ (R_1 = N-containing heterocyclic
group; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; R_4
= C3-10 hydrocarbyl; R_5-6 = C1-10 hydrocarbyl; $x = 1-2$; $y = 0-1$; z
= 2-3; $x + y + z = 4$). A catalyst component prepared by contacting

a solid prepared from G 952, BuMgEt, (EtO)₄Si, Cl₃CCH₂OH, TiCl₄, and di-Bu phthalate with propene in the presence of Et₃Al and 2,3,4-trimethyl-3-azacyclopentyltrimethoxysilane was used with Et₃Al and Ph₂Si(OMe)₂ for the **polymerization** of propene and the subsequent copolymn. of propene and ethylene, giving a block copolymer showing Young's flexural modulus 9500 kg/cm², Du Pont impact strength 62.7 kg-cm, and melt index 6.5.

IT 169544-35-8
(catalysts; for preparation of ethylene-propene block copolymers with impact resistance and rigidity)
RN 169544-35-8 HCAPLUS
CN 1H-Pyrrole, 2-(ethoxydimethoxysilyl)-2,5-dihydro-1-methyl- (9CI)
(CA INDEX NAME)



IC ICM C08F210-06
ICS C08F004-658
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 37
ST ethylene propene block copolymer impact strength; rigidity
toughness ethylene propene block copolymer; **polymn**
catalyst ethylene propene block copolymer
IT **Polymerization** catalysts
(block, for preparation of ethylene-propene block copolymers with impact resistance and rigidity)
IT 78-10-4, Tetraethoxysilane 84-74-2 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses 115-20-8, 2,2,2-Trichloroethanol 7550-45-0, Titanium tetrachloride, uses 62202-86-2, Butylethylmagnesium 155958-83-1, 2,3,4-Trimethyl-3-azacyclopentyltrimethoxysilane 155958-84-2 159328-46-8 169544-35-8
(catalysts; for preparation of ethylene-propene block copolymers with impact resistance and rigidity)

L63 ANSWER 16 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:630394 HCAPLUS

DOCUMENT NUMBER: 123:257793

TITLE: Preparation of polypropylene by multistage **polymerization**

INVENTOR(S): Taki, Noryuki; Nomura, Yasuo; Nakajima, Masashi; Ishihara, Takeshi; Ueki, Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 07090022

A2

19950404

JP 1993-239476

1993

0927

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PRIORITY APPLN. INFO.:

JP 1993-239476

1993

0927

<--

OTHER SOURCE(S):

MARPAT 123:257793

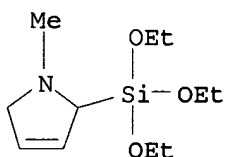
AB Title polypropylene with good melt flowability and workability are prepared by **polymerization** of propylene in the presence of **polymerization** catalysts obtained by treating olefins with solid catalysts containing metal oxides, Mg, Ti, halogens, and electron-donating compds. in the presence of organoaluminum compds. and $R_1xR_2ySi(OR_3)_z$ (R_1 = N-containing heterocyclic group; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; x = 1, 2; y = 0, 1; z = 2, 3; $x + y + z$ = 4; R_4 = C3-10 hydrocarbyl; R_5-6 = C1-10 hydrocarbyl), where melt flow rate (MFR) is 0.0001-10 g/10-min at the stage giving highest mol. weight and 10-1000 g/10-min at the stage giving lowest mol. weight. Thus, propylene were **polymerized** in the presence of a catalyst obtained by treating a solid catalyst containing G 952, Magala BEM, CCl_3CH_2OH , $TiCl_4$, and di-Bu phthalate with propylene in the presence of $AlEt_3$ and 2,3,4-trimethyl-3-azacyclopentyltrimethoxysilane at 70° for 1 h to give a polymer with MFR 0.7 at 1st stage, 89.4 at 2nd stage, and 18.0 g/10-min at final stage and flexural modulus 15,200 kg/cm².

IT 155958-85-3

(multistage preparation of polypropylene with good melt flowability and rigidity)

RN 155958-85-3 HCAPLUS

CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



IC ICM C08F010-06

ICS C08F004-658

CC 35-3 (Chemistry of Synthetic High Polymers)

ST propylene **polymn** catalyst heterocyclic silane; rigidity
polypropylene prepn catalyst; flowability melt polypropylene prepn catalyst

IT **Polymerization** catalysts

(multistage preparation of polypropylene with good melt flowability and rigidity)

IT 84-74-2, Dibutyl phthalate 93-89-0, Ethyl benzoate 97-93-8,
Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses
115-20-8, 2,2,2-Trichloroethanol 7550-45-0, Titanium
tetrachloride, uses 7631-86-9, G 952, uses 96119-56-1, Magala
BEM 155958-83-1, 2,3,4-Trimethyl-3-azacyclopentyltrimethoxysilan
e 155958-84-2 155958-85-3 159328-46-8

(multistage preparation of polypropylene with good melt flowability and rigidity)

L63 ANSWER 17 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1995:630391 HCAPLUS
 DOCUMENT NUMBER: 123:257791
 TITLE: Manufacture of propylene-ethylene copolymers
 with good rigidity and transparency
 INVENTOR(S): Ishihara, Takeshi; Ueki, Satoshi; Nakajima,
 Masashi; Taki, Noryuki; Nomura, Yasuo
 PATENT ASSIGNEE(S): Tonen Corp, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07090012	A2	19950404	JP 1993-239477	1993 0927

PRIORITY APPLN. INFO.:

JP 1993-239477

1993
0927

OTHER SOURCE(S): MARPAT 123:257791

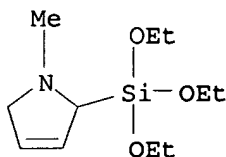
AB Propylene polymers containing 0.01-10% ethylene are prepared by using an olefin-pretreated **polymerization** catalyst comprising (1) a solid catalyst component containing metal oxides, Mg, Ti, halogens, and electron-donating compds., (2) an organoaluminum compound, and (3) silicon compound $R_1xR_2ySi(OR_3)z$ (R_1 = N-containing heterocycle; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; $x = 1, 2$; $y = 0, 1$; $z = 2, 3$; $x + y + z = 4$; R_4 = C3-10 hydrocarbyl; R_5-6 = C1-10 hydrocarbyl). Thus, ethylene and propylene were **polymerized** in the presence of a catalyst obtained by treating a solid catalyst containing G 952, Magala BEM, CCl_3CH_2OH , $TiCl_4$, and di-Bu phthalate with propylene in the presence of $AlEt_3$ and 2,3,4-trimethyl-3-azacyclopentyltrimethoxysilane at 70° for 1 h to give a copolymer with ethylene content 2.8%, melt flow rate 15.7 g/10-min, flexural modulus 10,790 kg/cm², and Haze 19.3%.

IT 155958-85-3

(manufacture of propylene-ethylene copolymers with good rigidity and transparency)

RN 155958-85-3 HCAPLUS

CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



(III)

IC ICM C08F004-658
 ICS C08F210-06

CC 35-3 (Chemistry of Synthetic High Polymers)
ST ethylene propylene polymn catalyst
IT Polymerization catalysts
(modified Ziegler-Natta, manufacture of propylene-ethylene copolymers with good rigidity and transparency)
IT 84-74-2, Dibutyl phthalate 93-89-0, Ethyl benzoate 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses 115-20-8, 2,2,2-Trichloroethanol 7550-45-0, Titanium tetrachloride, uses 7631-86-9, G 952, uses 96119-56-1, Magala BEM 155958-83-1, 2,3,4-Trimethyl-3-azacyclopentyltrimethoxysilane 155958-84-2 155958-85-3 159328-46-8
(manufacture of propylene-ethylene copolymers with good rigidity and transparency)

L63 ANSWER 18 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:422765 HCAPLUS

DOCUMENT NUMBER: 122:187562

TITLE: Preparation of 4,5-dihydro-4,5-dihydroxyphthalic acid ketal anhydrides as monomers

INVENTOR(S): Ueda, Mitsuru; Oota, Katsu; Matsubara, Minoru; Fujiwara, Hideetsu

PATENT ASSIGNEE(S): Japan Synthetic Rubber Co Ltd, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

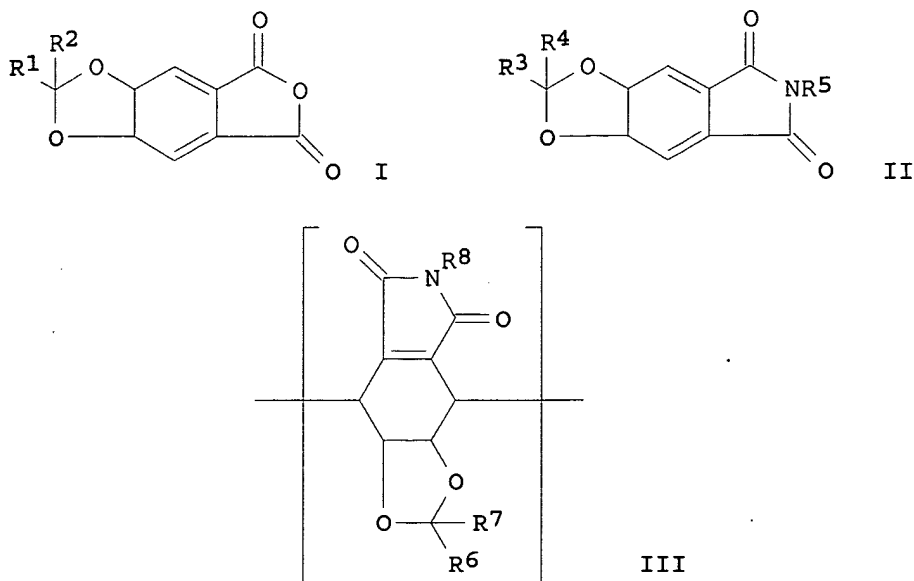
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06321949	A2	19941122	JP 1993-132648	1993 0510

PRIORITY APPLN. INFO.: <-- JP 1993-132648

1993
0510

OTHER SOURCE(S): CASREACT 122:187562; MARPAT 122:187562

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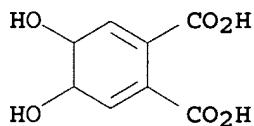
AB Title compds. I [R1, R2 = H, aliphatic hydrocarbyl, aromatic hydrocarbyl] and the imides II [R3, R4 = H, aliphatic hydrocarbyl, aromatic hydrocarbyl; R5 = (un)substituted aliphatic hydrocarbyl, aromatic hydrocarbyl] are prepared for the synthesis of the polymers III [R6, R7 = H, aliphatic hydrocarbyl, aromatic hydrocarbyl; R8 = (un)substituted aliphatic hydrocarbyl, aromatic hydrocarbyl] with an average mol. weight of 1,000-500,000. Thus, 4,5-dihydro-4,5-dihydroxyphthalic acid was treated with p-toluenesulfonic monohydrate and acetone at room temperature for 4 h to give 4,5-dihydro-4,5-dihydroxyphthalic anhydride ketal. This was reacted with p-butylaniline to give II [R3 = R4 = H, R5 = butyl], which was **polymerized** in the presence of dibenzoyl peroxide at 90° for 24 h to give 27% the corresponding polymer III with an average mol. weight of 3000-53,000.

IT 128666-29-5

(conversion into dihydrodihydroxyphthalic anhydride ketal)

RN 128666-29-5 HCAPLUS

CN 2,6-Cyclohexadiene-1,2-dicarboxylic acid, 4,5-dihydroxy- (9CI)
(CA INDEX NAME)



IC ICM C07D491-056

ICS C07D493-04; C08F022-40

CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 35

IT 128666-29-5

(conversion into dihydrodihydroxyphthalic anhydride ketal)

IT 161609-09-2P

(preparation and **polymerization** of)

L63 ANSWER 19 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:354750 HCAPLUS

DOCUMENT NUMBER: 122:291767

TITLE: Preparation of polypropene with good melt fluidity and rigidity by multistep **polymerization**

INVENTOR(S): Kanazawa, Seizaburo; Ookura, Masatoshi; Nakajima, Masashi; Ueki, Satoshi; Ishihara, Takeshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06298860	A2	19941025	JP 1993-87710	1993 0415

PRIORITY APPLN. INFO.:

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JP 1993-87710

1993
0415

OTHER SOURCE(S): MARPAT 122:291767

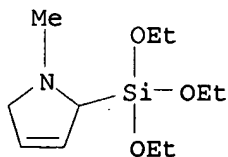
AB The title polymer (I) is prepared by multistep **polymerization** in the presence of catalysts comprising a solid containing Mg, Ti, halogen, and an electron donor, an organic Al compound, and a silane $R_1xSiR_2y(OR_3)z$ (R_1 = N-containing heterocyclic group; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; x = 1-2; y = 0-1; z = 2-3; $x + y + z = 4$; R_4 = C3-10 hydrocarbyl; R_5-6 = C1-10 hydrocarbyl), the melt index of I being controlled at 10-1000 and 0.0001-10, resp., in the steps giving the lowest and highest mol. weight A solid prepared from Mg, $BuMgCl$, $BuCl$, $HC(OEt)_3$, Cl_3CCH_2OH , $TiCl_4$, and di-Bu phthalate was used with Et_3Al , (2,3,4-trimethyl-3-azacyclopentyl)trimethoxysilane, and $Ph_2Si(OMe)_2$ for the 2-step **polymerization** of propene, giving I having flexural modulus 15,700 kg/cm².

IT 155958-85-3

(catalysts; for propene **polymerization** for controlled melt index)

RN 155958-85-3 HCAPLUS

CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



IC ICM C08F010-06
ICS C08F004-654
CC 35-3 (Chemistry of Synthetic High Polymers)
ST polypropene prepn catalyst melt index; rigidity polypropene prepn catalyst; silane **polymn** catalyst propene; **polymn** catalyst polypropene melt index
IT **Polymerization** catalysts
(modified Ziegler, for preparation of polypropene with controlled melt index and high rigidity)
IT 84-74-2, Dibutyl phthalate 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses 109-69-3, Butyl chloride 115-20-8, 2,2,2-Trichloroethanol 122-51-0 693-04-9, Butylmagnesium chloride 7439-95-4, Magnesium, uses 7550-45-0, Titanium tetrachloride, uses 155958-83-1 155958-84-2 **155958-85-3** 159328-46-8
(catalysts; for propene **polymerization** for controlled melt index)

L63 ANSWER 20 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:347260 HCAPLUS
DOCUMENT NUMBER: 122:291764
TITLE: Preparation of ethylene-propylene copolymers
INVENTOR(S): Ookura, Masatoshi; Kanazawa, Seizaburo; Nakajima, Masashi; Ishihara, Takeshi; Ueki, Satoshi
PATENT ASSIGNEE(S): Tonen Corp, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 06298833	A2	19941025	JP 1993-87555	1993 0414

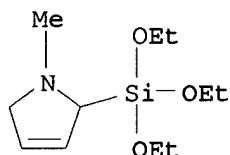
PRIORITY APPLN. INFO.: <-- JP 1993-87555
1993
0414

OTHER SOURCE(S): MARPAT 122:291764

AB The title copolymers containing 0.01-10% ethylene with good transparency and rigidity are prepared by **polymerization** of propylene and ethylene in the presence of catalysts obtained by treating olefins with (A) solid components containing Mg, Ti, halides, and electron-donating compds., (B) organic Al compds., and (C) (R1)x(R2)ySi(OR3)z (R1 = N-containing heterocyclic group; R2 = C1-10 hydrocarbyl, R4O, R5Si, R6SiO; R3 = Me, Et; x = 1, 2; y = 0, 1; z = 2, 3; x + y + z = 4; R4 = C3-10 hydrocarbyl; R5-6 = C1-10 hydrocarbyl). Thus, ethylene and propylene were **polymerized** in the presence of catalysts containing a solid catalyst obtained from Mg, MgBuCl, BuCl, CCl3CH2OH, TiCl4, and di-Bu phthalate, AlEt3, 2,3,4-trimethyl-3-azacyclopentyltrimethoxysilane, and Ph2Si(OMe)2 at 70° for 1 h to give a copolymer with ethylene content 3.8%, flexural modulus 10,860 kg/cm2, and Haze 18.9%.
IT **155958-85-3**

(catalysts for manufacture of ethylene-propylene copolymers with good transparency and rigidity)

RN 155958-85-3 HCAPLUS
CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



IC ICM C08F004-658
ICS C08F210-16
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 67
ST ethylene propylene **polymn** catalyst; dibutyl phthalate catalyst ethylene propylene **polymn**; chloroethanol catalyst ethylene propylene **polymn**; butyl chloride catalyst ethylene propylene **polymn**; aluminum catalyst ethylene propylene **polymn**; electron donor catalyst ethylene propylene **polymn**; halide catalyst ethylene propylene **polymn**; titanium catalyst ethylene propylene **polymn**; magnesium catalyst ethylene propylene **polymn**; silane **polymn** catalyst ethylene propylene; rigidity ethylene propylene copolymer prepn; transparency ethylene propylene copolymer prepn
IT **Polymerization** catalysts
(catalysts for manufacture of ethylene-propylene copolymers with good transparency and rigidity)
IT 84-74-2, Dibutyl phthalate 93-89-0, Ethyl benzoate 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses 109-69-3, Butyl chloride 115-20-8, 2,2,2-Trichloroethanol 693-04-9, Butylmagnesium chloride 6843-66-9, Dimethoxydiphenylsilane 7439-95-4, Magnesium, uses 7550-45-0, Titanium tetrachloride, uses 155958-83-1, 2,3,4-Trimethyl-3-azacyclopentyltrimethoxysilane 155958-84-2 **155958-85-3** 159328-46-8
(catalysts for manufacture of ethylene-propylene copolymers with good transparency and rigidity)

L63 ANSWER 21 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:339385 HCAPLUS

DOCUMENT NUMBER: 122:106769

TITLE: α -Olefin **polymerization**
catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity

INVENTOR(S): Ishihara, Takeshi; Kanazawa, Seizaburo; Imanishi, Kunihiro; Nakajima, Masashi; Ueki, Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06157649	A2	19940607	JP 1992-306813	1992 1117

PRIORITY APPLN. INFO.: JP 1992-306813
1992
1117

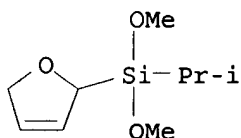
OTHER SOURCE(S): MARPAT 122:106769

AB The title components are formed by contacting a solid component containing Mg, Ti, halogen, and electron donor, with an olefin in the presence of organoaluminum compds. and organosilicon compds. R1aR2bSi(OR3)c (R1 = O- or S-containing cyclic residue; R2 = C1-10 hydrocarbyl, R4O, R5Si, R6SiO; R3 = Me, Et; a = 1, 2; b = 0, 1; c = 2, 3; a + b + c = 4; R4 = C3-10 hydrocarbyl; R5, R6 = C1-10 hydrocarbyl). A component was prepared from Mg, Bu2O, BuMgCl, BuCl, Et orthoformate, Cl3CCH2OH, TiCl4, and di-Bu phthalate, treated with propylene in the presence of Et3Al and bis(3-tetrahydrofuryl)dimethoxysilane and used together with Et3Al and diphenyldimethoxysilane for **polymerization** of propylene with catalyst efficiency 41.8 kg polymer/g-catalyst component-h and heptane-insol. content 97.8%.

IT 160245-98-7
(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)

RN 160245-98-7 HCAPLUS

CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethyl)- (9CI)
(CA INDEX NAME)



IC ICM C08F010-00
ICS C08F004-658

CC 35-3 (Chemistry of Synthetic High **Polymers**)

ST magnesium catalyst olefin **polymn**; titanium catalyst olefin **polymn**; electron donor catalyst olefin **polymn**; silane catalyst olefin **polymn**; polypropylene manuf catalyst

IT **Polymerization** catalysts
(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)

IT Silanes
(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)

IT Alkenes, preparation

(polymers, olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)

IT 84-74-2, Dibutyl phthalate 93-89-0, Ethyl benzoate 97-93-8, Triethylaluminum, uses 109-69-3, Butyl chloride 115-07-1, 1-Propene, uses 115-20-8, 2,2,2-Trichloroethanol 122-51-0, Ethyl orthoformate 142-96-1, Dibutyl ether 780-69-8, Phenyltriethoxysilane 6843-66-9, Dimethoxydiphenylsilane 7439-95-4, Magnesium, uses 7550-45-0, Titanium tetrachloride, uses 158069-53-5 158069-54-6 158069-55-7 158069-56-8 158069-57-9 159412-70-1 **160245-98-7**

(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)

IT 9003-07-0P, Polypropylene

(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)

L63 ANSWER 22 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:339384 HCAPLUS

DOCUMENT NUMBER: 122:106768

TITLE: α -Olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity

INVENTOR(S): Furuhashi, Hiroyuki; Imanishi, Kunihiro; Taki, Noryuki; Ueki, Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06157650	A2	19940607	JP 1992-306814	1992 1117

PRIORITY APPLN. INFO.: <-- JP 1992-306814

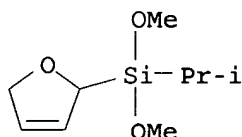
1992
1117

OTHER SOURCE(S): MARPAT 122:106768

AB The title components are formed by contacting a solid component containing metal oxide, Mg, Ti, halogen, and electron donor, with an olefin in the presence of organoaluminum compds. and organosilicon compds. R1aR2bSi(OR3)c (R1 = O- or S-containing cyclic residue; R2 = C1-10 hydrocarbyl, R4O, R5Si, R6SiO; R3 = Me, Et; a = 1, 2; b = 0, 1; c = 2, 3; a + b + c = 4; R4 = C3-10 hydrocarbyl; R5, R6 = C1-10 hydrocarbyl). A component was prepared from G-952, BuMgEt, Si(OEt)4, Cl3CCH2OH, TiCl4, and di-Bu phthalate, treated with propylene in the presence of Et3Al and bis(3-tetrahydrofuryl)dimethoxysilane and used together with Et3Al and diphenyldimethoxysilane for **polymerization** of propylene with

catalyst efficiency 41.8 kg polymer/g-catalyst component-h and heptane-insol. content 97.8%.

- IT 160245-98-7
(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)
- RN 160245-98-7 HCAPLUS
- CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethyl)- (9CI)
(CA INDEX NAME)



- IC ICM C08F010-00
ICS C08F004-658
- CC 35-3 (Chemistry of Synthetic High Polymers)
- ST magnesium catalyst olefin **polymn**; titanium catalyst olefin **polymn**; electron donor catalyst olefin **polymn**; silane catalyst olefin **polymn**; polypropylene manuf catalyst; silica catalyst olefin **polymn**
- IT **Polymerization** catalysts
(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)
- IT Silanes
(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)
- IT Alkenes, preparation
(polymers, olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)
- IT 78-10-4 84-74-2, Dibutyl phthalate 93-89-0, Ethyl benzoate 97-93-8, Triethylaluminum, uses 115-07-1, 1-Propene, uses 115-20-8, 2,2,2-Trichloroethanol 780-69-8, Phenyltriethoxysilane 6843-66-9, Dimethoxydiphenylsilane 7550-45-0, Titanium tetrachloride, uses 7631-86-9, Silica, uses 62202-86-2, ButylethylMagnesium 158069-53-5 158069-54-6 158069-55-7 158069-56-8 158069-57-9 159412-70-1 160245-98-7
(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)
- IT 9003-07-0P, Polypropylene
(olefin **polymerization** catalyst components providing increased catalyst particle strength, activity retention, and storability and polymer rigidity)

L63 ANSWER 23 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:331297 HCAPLUS

DOCUMENT NUMBER: 122:266318

TITLE: Catalysts for preparation of propene block copolymers

INVENTOR(S): Nakajima, Masashi; Ueki, Satoshi; Ishihara, Takeshi; Ookura, Masatoshi; Kanazawa,

Seizaburo
 PATENT ASSIGNEE(S): Tonen Corp, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06298830	A2	19941025	JP 1993-87556	

1993
0414

PRIORITY APPLN. INFO.:

<--
JP 1993-87556

1993
0414

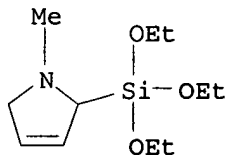
OTHER SOURCE(S): MARPAT 122:266318

AB Block copolymers with good impact strength and rigidity and highly crystalline propene polymers are prepared by using catalysts obtained by treating olefins with solid components containing Mg, Ti, halogen, and electron donor compds., organic Al compds., and silanes $R_1xSiR_2y(OR_3)z$ (R_1 = N-containing heterocyclic group; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; x = 1-2; y = 0-1; z = 2-3; $x + y + z = 4$; R_4 = C3-10 hydrocarbyl; R_5-6 = C1-10 hydrocarbyl). Propene was polymerized in the presence of a solid prepared from Mg, $BuMgCl$, $BuCl$, Cl_3CCH_2OH , $TiCl_4$, and di-Bu phthalate, Et_3Al , 2,3,4-trimethyl-3-azacyclopentyltrimethoxysilane, and $Ph_2Si(OMe)_2$ at 70° for 1 h, followed by polymerization of propene and ethylene at 75° for 1.5 h to give a block copolymer with flexural modulus 7740 kg/cm² and impact strength 104.5 kg-cm.

IT 155958-85-3
 (catalysts; for block polymerization of propene and ethylene)

RN 155958-85-3 HCAPLUS

CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



IC ICM C08F004-654

ICS C08F210-16; C08F297-08

CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 37

ST ethylene propene block polymn catalyst; impact resistance ethylene propene copolymer; rigidity ethylene propene block copolymer; polypropene crystallinity polymn catalyst

IT Silanes

(catalysts; for block polymerization of propene and ethylene)

IT **Polymerization catalysts**

(block, for ethylene and propene)

IT 84-74-2, Dibutyl phthalate 93-89-0, Ethyl benzoate 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses 109-69-3, Butyl chloride 115-20-8, 2,2,2-Trichloroethanol 693-04-9, Butylmagnesium chloride 7439-95-4, Magnesium, uses 7550-45-0, Titanium tetrachloride, uses 155958-83-1 155958-84-2 **155958-85-3** 159328-46-8

(catalysts; for block polymerization of propene and ethylene)

L63 ANSWER 24 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:330538 HCAPLUS

DOCUMENT NUMBER: 122:106766

TITLE: Stereospecific α -olefin polymerization catalysts

INVENTOR(S): Ueki, Satoshi; Aoki, Tomoko; Imanishi, Kunihiro; Ishihara, Takeshi; Taki, Noryuki; Saito, Hiroo

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06145235	A2	19940524	JP 1991-247587	1991 0926

PRIORITY APPLN. INFO.: <-- JP 1991-247587

1991
0926

<--

OTHER SOURCE(S): MARPAT 122:106766

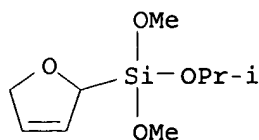
AB The title catalysts comprise (A) a solid component containing metal oxide, Mg, Ti, halogen, and electron donor, (B) organometallic compds. and (C) organosilicon compds. $R_1aR_2bSi(OR_3)c$ ($R_1 = O-$ or S-containing cyclic residue; $R_2 = C_1-10$ hydrocarbyl, R_4O , R_5Si , R_6SiO ; $R_3 = Me$, Et ; $a = 1, 2$; $b = 0, 1$; $c = 2, 3$; $a + b + c = 4$; $R_4 = C_3-10$ hydrocarbyl; $R_5, R_6 = C_1-10$ hydrocarbyl). A component was prepared from G-952, $BuMgEt$, $Si(OEt)_4$, Cl_3CCH_2OH , $TiCl_4$, and di-Bu phthalate and used together with Et_3Al and bis(3-tetrahydrofuryl)dimethoxysilane for polymerization of propylene with catalyst efficiency 16.7 kg polymer/g-catalyst component A and heptane-insol. content 96.8%.

IT 158069-58-0

(stereospecific α -olefin polymerization catalysts)

RN 158069-58-0 HCAPLUS

CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethoxy)- (9CI)
(CA INDEX NAME)



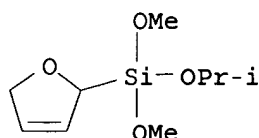
IC ICM C08F010-00
ICS C08F004-658
CC 35-3 (Chemistry of Synthetic High Polymers)
ST magnesium catalyst olefin **polymn**; titanium catalyst
olefin **polymn**; electron donor catalyst olefin
polymn; silane catalyst olefin **polymn**;
polypropylene manuf catalyst; silica catalyst olefin
polymn
IT **Polymerization catalysts**
(stereospecific α -olefin **polymerization catalysts**)
IT Silanes
(stereospecific α -olefin **polymerization catalysts**)
IT Alkenes, preparation
(polymers, stereospecific α -olefin **polymerization**
catalysts)
IT 78-10-4 84-74-2, Dibutyl phthalate 97-93-8, Triethylaluminum,
uses 115-20-8, 2,2,2-Trichloroethanol 7550-45-0, Titanium
tetrachloride, uses 7631-86-9, Silica, uses 62202-86-2,
ButylethylMagnesium 158069-53-5 158069-54-6 158069-56-8
158069-57-9 **158069-58-0**
(stereospecific α -olefin **polymerization catalysts**)
IT 9003-07-0P, Polypropylene
(stereospecific α -olefin **polymerization catalysts**)

L63 ANSWER 25 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:231107 HCAPLUS
DOCUMENT NUMBER: 122:10949
TITLE: Highly stereospecific α -olefin
polymerization catalysts containing
nonaromatic organosilicon compounds
INVENTOR(S): Usui, Myuki; Imanishi, Kunihiko; Ishihara,
Takeshi; Ueki, Satoshi
PATENT ASSIGNEE(S): Tonen Corp, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06136042	A2	19940517	JP 1992-291451	1992 1029
PRIORITY APPLN. INFO.: JP 1992-291451				1992 1029

OTHER SOURCE(S): MARPAT 122:10949

- AB The catalysts comprise activated TiCl_3 , organometallic compds., and organic Si compds. $\text{R}_1\text{aR}_2\text{bSi}(\text{OR}_3)_c$ [R_1 = cyclic (thio)ether residue; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; $a = 1, 2$; $b = 0, 1$; $c = 2, 3$; $a + b + c = 4$; R_4 = C3-10 hydrocarbyl; R_5, R_6 = C1-10 hydrocarbyl], e.g., bis(tetrahydrofuran-3-yl)dimethoxysilane, tetrahydrofuran-3-yltriethoxysilane, tetrahydropyran-4-yltrimethoxysilane, dimethoxy(tetrahydropyran-4-yl)(trimethylsiloxy)silane, etc. A polypropylene obtained had heptane-insol. content 98.1% with catalyst efficiency 6.0 kg polymer/g TiCl_3 .
- IT **158069-58-0**
(highly stereospecific α -olefin **polymerization**
catalysts containing nonarom. organosilicon compds.)
- RN 158069-58-0 HCAPLUS
- CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethoxy) - (9CI)
(CA INDEX NAME)



- IC ICM C08F010-00
ICS C08F004-64
- CC 35-3 (Chemistry of Synthetic High **Polymers**)
- ST silane catalyst olefin **polymn**; titanium trichloride catalyst olefin **polymn**; polypropylene stereoregular **polymn** catalyst
- IT Silanes
(highly stereospecific α -olefin **polymerization**
catalysts containing nonarom. organosilicon compds.)
- IT Alkenes, preparation
(polymers, highly stereospecific α -olefin **polymn**
. catalysts containing nonarom. organosilicon compds.)
- IT **Polymerization** catalysts
(stereospecific, highly stereospecific α -olefin
polymerization catalysts containing nonarom. organosilicon compds.)
- IT 96-10-6, Diethylaluminum chloride, uses 97-93-8, Triethylaluminum, uses 142-96-1, Dibutyl ether 7550-45-0, Titanium tetrachloride, uses 7705-07-9, Titanium trichloride, uses 158069-53-5 158069-54-6 158069-55-7 158069-56-8 158069-57-9 **158069-58-0**
(highly stereospecific α -olefin **polymerization**
catalysts containing nonarom. organosilicon compds.)
- IT 9003-07-0P, Polypropylene
(highly stereospecific α -olefin **polymerization**
catalysts containing nonarom. organosilicon compds.)

L63 ANSWER 26 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:137136 HCAPLUS

DOCUMENT NUMBER: 122:134151

TITLE: Preparation of polypropylene using cyclic ether-having silane catalysts

INVENTOR(S): Taki, Noryuki; Nakajima, Masashi; Furuhashi, Hiroyuki; Imanishi, Kunihiro; Ueki, Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

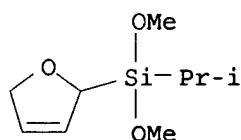
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06211930	A2	19940802	JP 1993-5816	1993 0118

PRIORITY APPLN. INFO.: JP 1993-5816
 1993
 0118

OTHER SOURCE(S): MARPAT 122:134151

AB Polypropylene is prepared by multistage **polymerization** in the presence of catalysts obtained by contacting (A) solid catalysts containing metal oxides, Mg, Ti, halogen, and electron-donating compds., (B) organic Al compds., (C) $R_1xR_2ySi(OR_3)z$ ($R_1 = O-$ or S-containing cyclic group; $R_2 = C_1-10$ hydrocarbyl, R_4O , R_5Si , R_6SiO ; $R_3 = Me$, Et ; $R_4 = C_3-10$ hydrocarbyl; $R_5-6 = C_1-10$ hydrocarbyl; $x = 1, 2$; $y = 0, 1$; $z = 2, 3$; $x + y + z = 4$), and (D) olefins, where polypropylene obtained at each stage has different melt flow rate (MFR) and MFR is 0.0001-10 g/10-min and 10-1000 g/10-min at the stage giving the highest or lowest mol.-weight polypropylene, resp. Thus, propylene was prepolymerized in the presence of a solid catalyst obtained from G 952, $BuEtMg$, Cl_3CCH_2OH , $TiCl_4$, and di-Bu phthalate, Et_3Al , and bis(oxacyclopent-3-yl)dimethoxysilane and then **polymerized** with Et_3Al and $Ph_2(OMe)_2Si$ to give polypropylene with MFR 25.0 g/10-min, catalytic activity 9.8 kg/g-solid catalyst-h, and flexural modulus $15.1 + 103$ kg/cm².

IT 160245-98-7
 (aluminum-magnesium-titanium-cyclic ether-containing silane-metal oxide catalysts for multistage **polymerization** of propylene)
 RN 160245-98-7 HCAPLUS
 CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethyl)- (9CI)
 (CA INDEX NAME)



IC ICM C08F010-06
 ICS C08F004-658
 CC 35-3 (Chemistry of Synthetic High Polymers)
 ST propylene **polymn** multistage catalyst; aluminum magnesium titanium catalyst **polymn** propylene; cyclic ether silane catalyst prepolypropylene; oxide metal catalyst **polymn** propylene; thioether cyclic silane catalyst propylene **polymn**; chloroethanol catalyst propylene **polymn**; phthalate catalyst propylene **polymn**; phenyl

- dimethoxysilane catalyst propylene **polymn**;
 oxacyclopentyl dimethoxysilane catalyst propylene **polymn**
- IT Electron donors
 Polymerization catalysts
 (aluminum-magnesium-titanium-cyclic ether-containing silane-metal
 oxide catalysts for multistage **polymerization** of propylene)
- IT Oxides, uses
 (aluminum-magnesium-titanium-cyclic ether-containing silane-metal
 oxide catalysts for multistage **polymerization** of propylene)
- IT Ethers, uses
 Sulfides, uses
 (cyclic, aluminum-magnesium-titanium-cyclic ether-containing
 silane-metal oxide catalysts for multistage **polymerization**
 of propylene)
- IT 84-74-2, Dibutyl phthalate 93-89-0, Ethyl benzoate 97-93-8,
 Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses
 115-20-8, 2,2,2-Trichloroethanol 6843-66-9,
 Diphenyldimethoxysilane 7550-45-0, Titanium tetrachloride, uses
 7631-86-9, G 952, uses 62202-86-2, Butylethylmagnesium
 158069-53-5 158069-54-6 158069-55-7 158069-56-8
 158069-57-9 159412-70-1 160245-98-7
 (aluminum-magnesium-titanium-cyclic ether-containing silane-metal
 oxide catalysts for multistage **polymerization** of propylene)
- IT 9003-07-0P, Polypropylene
 (aluminum-magnesium-titanium-cyclic ether-containing silane-metal
 oxide catalysts for multistage **polymerization** of propylene)

L63 ANSWER 27 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:137135 HCAPLUS

DOCUMENT NUMBER: 122:134150

TITLE: Preparation of polypropylene using cyclic
 ether-containing silane catalysts

INVENTOR(S): Ookura, Masatoshi; Kanazawa, Seizaburo;
 Ishihara, Takeshi; Imanishi, Kunihiro; Ueki,
 Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06211929	A2	19940802	JP 1993-5815	1993 0118

PRIORITY APPLN. INFO.: JP 1993-5815

1993
0118

OTHER SOURCE(S): MARPAT 122:134150

AB Polypropylene is prepared by multistage **polymerization** in the
 presence of catalysts obtained by contacting (A) solid catalysts
 containing Mg, Ti, halogen, and electron-donating compds., (B) organic Al
 compds., (C) $R_1xR_2ySi(OR_3)_z$ ($R_1 = O-$ or $S-$ -containing cyclic group; R_2
 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; $R_3 = Me$, Et ; $R_4 = C3-10$)

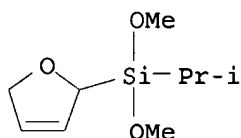
hydrocarbyl; R5-6 = C1-10 hydrocarbyl; x = 1, 2; y = 0, 1; z = 2, 3; x + y + z = 4), and (D) olefins, where polypropylene obtained at each stage has different melt flow rate (MFR) and MFR is 0.0001-10 g/10-min and 10-1000 g/10-min at the stage giving the highest or lowest mol.-weight polypropylene, resp. Thus, propylene was prepolymerized in the presence of a solid catalyst obtained from Mg, BuMgCl, BuCl, Cl₃CCH₂OH, TiCl₄, and di-Bu phthalate, Et₃Al, and bis(oxacyclopent-3-yl)dimethoxysilane and then polymerized with Et₃Al and Ph₂(OMe)₂Si to give polypropylene with MFR 18.9 g/10-min, catalytic activity 21.0 kg/g-solid catalyst-h, and flexural modulus 16.1 + 103 kg/cm².

IT 160245-98-7

(aluminum-magnesium-titanium-cyclic ether-containing silane catalysts for multistage polymerization of propylene)

RN 160245-98-7 HCAPLUS

CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethyl)- (9CI)
(CA INDEX NAME)



IC ICM C08F010-06

ICS C08F004-658

CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 37

ST propylene polymer multistage catalyst; butyl chloride catalyst propylene polymer; aluminum magnesium titanium catalyst polymer propylene; cyclic ether silane catalyst prepolypropylene; phenyl dimethoxysilane catalyst propylene polymer; oxacyclopentyl dimethoxysilane catalyst propylene polymer; phthalate catalyst propylene polymer; chloroethanol catalyst propylene polymer

IT Electron donors

Polymerization catalysts

(aluminum-magnesium-titanium-cyclic ether-containing silane catalysts for multistage polymerization of propylene)

IT Ethers, uses

Sulfides, uses

(cyclic, aluminum-magnesium-titanium-cyclic ether-containing silane catalysts for multistage polymerization of propylene)

IT 84-74-2, Dibutyl phthalate 93-89-0, Ethyl benzoate 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses 109-69-3, Butyl chloride 115-20-8, 2,2,2-Trichloroethanol 693-04-9, Butylmagnesium chloride 6843-66-9, Diphenyldimethoxysilane 7439-95-4, Magnesium, uses 7550-45-0, Titanium tetrachloride, uses 158069-53-5 158069-54-6 158069-55-7 158069-56-8 158069-57-9 159412-70-1
160245-98-7

(aluminum-magnesium-titanium-cyclic ether-containing silane catalysts for multistage polymerization of propylene)

IT 9003-07-0P, Polypropylene

(aluminum-magnesium-titanium-cyclic ether-containing silane catalysts for multistage polymerization of propylene)

L63 ANSWER 28 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:126331 HCAPLUS
 DOCUMENT NUMBER: 122:82322
 TITLE: Preparation of propylene block copolymers with
 balanced impact resistance and rigidity
 INVENTOR(S): Nakajima, Masashi; Imanishi, Kunihiro;
 Furuhashi, Hiroyuki; Taki, Noryuki; Ueki,
 Satoshi
 PATENT ASSIGNEE(S): Tonen Corp, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06192313	A2	19940712	JP 1992-344504	1992 1224

PRIORITY APPLN. INFO.: JP 1992-344504
 1992
 1224

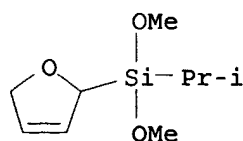
OTHER SOURCE(S): MARPAT 122:82322

AB Title process comprises (a) **polymerization** of highly crystalline polypropylene in the presence of **polymerization** catalysts prepared by contacting solids containing metal oxides, Mg, Ti, halogen, and electron donors with olefins in the presence of organic Al compds. and $R_1xR_2ySi(OR_3)z$ [R_1 = monovalent cyclic substituents having an ether or thioether bond in the ring; R_2 = C1-10 hydrocarbon residue, R_4O (R_4 = C3-10 hydrocarbon residue), R_5Si (R_5 = C1-10 hydrocarbon residue), R_6SiO (R_6 = R_5); R_3 = Me, Et; x = 1, 2; yr = 0, 1; z = 2, 3; $x + y + z = 4$] and (b) copolymn. of propylene (I) with ethylene (II). Thus, I was prepolymd. at 5° for 3.0 h in heptane (III) in the presence of 3.2 g of a solid prepared from G 952 (SiO_2), MAGALA BEM (20% BuEtMg III solution), $(EtO)_4Si$, $TiCl_4$, and DBP, 50 mmol/L-III Et_3Al , and 10 mmol/L-III bis(3-oxacyclopentyl)dimethoxysilane then liquid I was **polymerized** at 70° for 1 h in the presence of 120 mg of the product, Et_3Al and diphenyldimethoxysilane followed by copolymn. of I and II at 75° for 2 h to obtain 50:50 II-I block copolymer showing flexural modulus $8.39 + 103$ kg/cm² and duPont impact strength 87.1 kg-cm.

IT 160245-98-7
 (polymerization catalysts for preparation of propylene block copolymers with balanced impact resistance and rigidity)

RN 160245-98-7 HCAPLUS

CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethyl)- (9CI)
 (CA INDEX NAME)



IC ICM C08F004-658
ICS C08F210-16; C08F297-08
CC 35-4 (Chemistry of Synthetic High Polymers)
ST impact resistance propylene block copolymer; ethylene block
copolymer impact resistance; rigidity ethylene propylene block
copolymer; silica solid catalyst component prepn; butylethyl
magnesium solid catalyst component; titanium chloride solid
catalyst component; DBP solid catalyst component prepn;
ethylaluminum alkoxysilane **polymn** catalyst
IT Impact-resistant materials
Polymerization catalysts
(**polymerization** catalysts for preparation of propylene block
copolymers with balanced impact resistance and rigidity)
IT 84-74-2, DBP
(electron donors; **polymerization** catalysts for preparation of
propylene block copolymers with balanced impact resistance and
rigidity)
IT 9003-07-0P, Polypropylene
(highly crystalline; **polymerization** catalysts for preparation of
propylene block copolymers with balanced impact resistance and
rigidity)
IT 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum,
uses 7550-45-0, Titanium(IV) chloride, uses 7631-86-9, G 952,
uses 96119-56-1, MAGALA BEM 158069-53-5 158069-54-6
158069-55-7 158069-56-8 158069-57-9 159412-70-1
160245-98-7
(**polymerization** catalysts for preparation of propylene block
copolymers with balanced impact resistance and rigidity)
IT 106565-43-9P, Ethylene-propylene block copolymer
(**polymerization** catalysts for preparation of propylene block
copolymers with balanced impact resistance and rigidity)

L63 ANSWER 29 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:126330 HCAPLUS

DOCUMENT NUMBER: 122:82321

TITLE: Preparation of propylene block copolymers with
balanced impact resistance and rigidity

INVENTOR(S): Kanazawa, Seizaburo; Imanishi, Kunihiko;
Ishihara, Takeshi; Ookura, Masatoshi; Ueki,
Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 06192312	A2	19940712	JP 1992-344503	1992 1224

PRIORITY APPLN. INFO.:

<--
JP 1992-344503

1992
1224

<--

OTHER SOURCE(S): MARPAT 122:82321

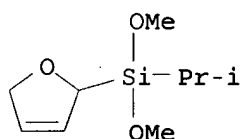
AB Title process comprises (a) **polymerization** of highly crystalline polypropylene in the presence of **polymerization** catalyst components prepared by contacting solids containing Mg, Ti, halogen, and electron donors with olefins in the presence of organic Al compds. and $R_1xR_2ySi(OR_3)_z$ [R_1 = monovalent cyclic substituents having an ether or thioether bond in the ring; R_2 = C1-10 hydrocarbon residue, R_4O (R_4 = C3-10 hydrocarbon residue), R_5Si (R_5 = C1-10 hydrocarbon residue), R_6SiO (R_6 = R_5); R_3 = Me, Et; $x = 1, 2$; $yr = 0, 1$; $z = 2, 3$; $x + y + z = 4$] and (b) copolymn. of propylene (I) with ethylene (II). Thus, I was prepolymd. at -5° for 2.0 h in heptane (III) in the presence of 3.5 g of a solid prepared from Mg, $BuMgCl$, $BuCl$, $HC(OEt)_3$, $TiCl_4$, and DBP, 50 mmol/L-III Et_3Al , and 10 mmol/L-III bis(3-oxacyclopentyl)dimethoxysilane to prepare a **polymerization** catalyst (B) then I was **polymerized** at 70° for 1 h in the presence of 49 mg B, Et_3Al , and diphenyldimethoxysilane followed by copolymd. with I and II at 75° for 2 h to obtain 49:51 II-I block copolymer showing flexural modulus 8.28 + 103 kg/cm² and du Pont impact strength 95.0 kg-cm.

IT 160245-98-7

(**polymerization** catalysts for preparation of propylene block copolymers with balanced impact resistance and rigidity)

RN 160245-98-7 HCAPLUS

CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethyl)- (9CI)
(CA INDEX NAME)



IC ICM C08F004-658

ICS C08F210-16; C08F297-08

CC 35-4 (Chemistry of Synthetic High Polymers)

ST impact resistance propylene block copolymer; ethylene block copolymer impact resistance; rigidity ethylene propylene block copolymer; metallic magnesium solid catalyst component; butylmagnesium chloride solid catalyst component; butyl chloride solid catalyst component; titanium chloride solid catalyst component; DBP solid catalyst component prepn; ethyl aluminum **polymn** catalyst component; bisoxacyclopentyldimethoxysilane **polymn** catalyst component

IT **Polymerization** catalysts

(**polymerization** catalysts for preparation of propylene block copolymers with balanced impact resistance and rigidity)

IT 84-74-2, DBP

(electron donors; **polymerization** catalysts for preparation of propylene block copolymers with balanced impact resistance and rigidity)

IT 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses 109-69-3, Butyl chloride 693-04-9, Butylmagnesium chloride 7429-90-5D, Aluminum, organic compds. 7439-95-4, Magnesium, uses 7440-21-3D, Silicon, organic compds. 158069-53-5 158069-54-6 158069-55-7 158069-56-8 158069-57-9 159412-70-1 160245-98-7

(**polymerization** catalysts for preparation of propylene block

copolymers with balanced impact resistance and rigidity)
 IT 7550-45-0, Titanium(IV) chloride, reactions
 (polymerization catalysts for preparation of propylene block
 copolymers with balanced impact resistance and rigidity)

L63 ANSWER 30 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

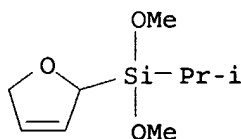
ACCESSION NUMBER: 1995:103612 HCAPLUS
 DOCUMENT NUMBER: 122:56810
 TITLE: Catalysts for preparation of transparent rigid
 ethylene-propene copolymers
 INVENTOR(S): Nakajima, Masashi; Imanishi, Kunihiro;
 Furuhashi, Hiroyuki; Taki, Noryuki; Ueki,
 Satoshi
 PATENT ASSIGNEE(S): Tonen Corp, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06192339	A2	19940712	JP 1992-342543	1992 1222

PRIORITY APPLN. INFO.: <-- JP 1992-342543
 1992
 1222

AB The title copolymers containing 0.01-10% ethylene are prepared with catalysts prepared by treating solid components containing metal oxides, Mg, Ti, halogens, and electron donors with olefins in the presence of organic Al compds. and silanes R₁SiR₂y(OR₃)_z [R₁ = (thio)ether bond-containing cyclic group; R₂ = C₁-10 hydrocarbyl, OR₄, SiR₅3, OSiR₆3; R₃ = Me, Et; R₄ = C₃-10 hydrocarbyl; R₅-6 = C₁-10 hydrocarbyl; x = 1-2; y = 0-1; z = 2-3; x + y + z = 4]. A solid prepared from G 952, Magala BEM (BuEtMg/heptane), Si(OEt)₄, Cl₃CCH₂OH, TiCl₄, and di-Bu phthalate was used with AlEt₃ and (MeO)₂SiR₇2 (R₇ = oxacyclopent-3-yl) for the polymerization of propene, giving a catalyst component which was used with AlEt₃ and Ph₂SiMe₂ for the copolymn. of propene and ethylene in heptane under H at 70° to give a copolymer showing melt index 15.2, ethylene content 2.6%, flexural modulus 10,660 kg/cm², and haze 19.6%.

IT 160245-98-7
 (catalysts; for copolymn. of ethylene and propene)
 RN 160245-98-7 HCAPLUS
 CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethyl)- (9CI)
 (CA INDEX NAME)



IC ICM C08F210-06
ICS C08F004-658
CC 35-3 (Chemistry of Synthetic High Polymers)
ST propene ethylene copolymn catalyst; **polymn** catalyst
ethylene propene; magnesium catalyst copolymn propene ethylene;
titanium catalyst copolymn propene ethylene; aluminum catalyst
copolymn propene ethylene; silane catalyst copolymn propene
ethylene; transparency ethylene propene copolymer prepn
IT **Polymerization** catalysts
(for ethylene and propene as rigid transparent copolymers)
IT 78-10-4, Tetraethoxysilane 84-74-2, Dibutyl phthalate 97-93-8,
Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses
115-20-8, 2,2,2-Trichloroethanol 7550-45-0, Titanium
tetrachloride, uses 62202-86-2, Butylethylmagnesium
96119-56-1, Butylethylmagnesium 158069-53-5 158069-54-6
158069-55-7 158069-56-8 158069-57-9 159412-70-1
160245-98-7
(catalysts; for copolymn. of ethylene and propene)

L63 ANSWER 31 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:103611 HCAPLUS
DOCUMENT NUMBER: 122:106796
TITLE: Manufacture of transparent rigid propylene
copolymers
INVENTOR(S): Kanazawa, Seizaburo; Imanishi, Kunihiro;
Ishihara, Takeshi; Ookura, Masatoshi; Ueki,
Satoshi
PATENT ASSIGNEE(S): Tonen Corp, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06192338	A2	19940712	JP 1992-342542	1992 1222

PRIORITY APPLN. INFO.: JP 1992-342542
1992
1222

OTHER SOURCE(S): MARPAT 122:106796

AB Ethylene-propylene copolymers with 0.01-10% ethylene content are
manufactured with catalysts prepared by treating solid components containing
Mg, Ti, halogens, and electron donors with olefins in the presence
of organoaluminum compds. and (R1)x(R2)ySi(OR3)z [R1 = (thio)ether
bond-containing cyclic group; R2 = C1-10 hydrocarbyl, OR4, Si(R5)3,
OSi(R6)3; R3 = Me, Et; R4 = C3-10 hydrocarbyl; R5-6 = C1-10
hydrocarbyl; x = 1, 2; y = 0, 1; z = 2, 3; x + y + z = 4]. Thus,
a mixture of a component [prepared from Mg, BuMgCl, BuCl, HC(OEt)3,
Cl3CCH2OH, TiCl4, and di-Bu phthalate], AlEt3, and
bis(oxacyclopent-3-yl)dimethoxysilane was prepolymd. with
propylene to prepare a catalyst component, which was mixed with
AlEt3 and Ph2SiMe2 and used in copolymn. of propylene and ethylene

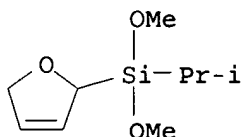
in n-heptane under H at 70° for 1 h to give a polymer showing melt flow rate 15.2 g/10 min, ethylene content 2.0%, flexural modulus 11.04 + 103 kg/cm², and haze 22.1%.

IT 160245-98-7

(catalysts for manufacture of transparent and rigid propylene-ethylene copolymer)

RN 160245-98-7 HCAPLUS

CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethyl)- (9CI)
(CA INDEX NAME)



IC ICM C08F210-06

ICS C08F004-658

CC 35-4 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67

IT **Polymerization** catalysts

(catalysts for manufacture of transparent and rigid propylene-ethylene copolymer)

IT 84-74-2, Dibutyl phthalate 97-93-8, Triethylaluminum, uses
100-99-2, Triisobutylaluminum, uses 109-69-3, Butyl chloride
115-20-8, 2,2,2-Trichloroethanol 122-51-0, Triethoxymethane
693-04-9, Butylmagnesium chloride 7439-95-4, Magnesium, uses
7550-45-0, Titanium tetrachloride, uses 158069-53-5
158069-54-6 158069-55-7 158069-56-8 158069-57-9
159412-70-1 **160245-98-7**

(catalysts for manufacture of transparent and rigid propylene-ethylene copolymer)

L63 ANSWER 32 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:79185 HCAPLUS

DOCUMENT NUMBER: 122:10955

TITLE: Catalysts for polymerization of α -olefins

INVENTOR(S): Nakajima, Masashi; Furuhashi, Hiroyuki; Taki, Noryuki; Imanishi, Kunihiro; Ueki, Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06179718	A2	19940628	JP 1992-331459	1992 1211

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PRIORITY APPLN. INFO.: JP 1992-331459

1992
1211

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OTHER SOURCE(S): MARPAT 122:10955

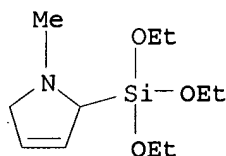
AB The title catalysts, giving polymers with high stiffness, are prepared by contacting olefins with organic Al compds., solid components containing metal oxides, Mg, Ti, halo compds., and electron donors, and silanes $R_1xSiR_2y(OR_3)z$ (R_1 = N-containing heterocyclic group; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; R_4 = C3-10 hydrocarbyl; R_5-6 = C1-10 hydrocarbyl; $x = 1-2$; $y = 0-1$; $z = 2-3$; $x + y + z = 4$). Propene was prepolymd. in the presence of Et_3Al , a solid component prepared from G 952, $BuMgEt$, Cl_3CCH_2OH , $TiCl_4$, and di-Bu phthalate, and 1,2,5-trimethyl-3-(trimethoxysilyl)pyrrolidine to give a catalyst which was used to polymerize propene, giving 15.5 kg polypropene/g solid catalyst component/h.

IT 155958-85-3

(catalysts; for polymerization of α -olefins)

RN 155958-85-3 HCAPLUS

CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



IC ICM C08F010-00

ICS C08F004-658

CC 35-3 (Chemistry of Synthetic High Polymers)

ST aluminum catalyst polymn olefin; titanium catalyst polymn olefin; silane catalyst polymn olefin; pyrrole deriv catalyst polymn olefin; polypropene polymn catalyst

IT Polymerization catalysts

(aluminum compound-titanium compound-silane derivative, for α -olefins)

IT Silanes

(alkoxy, cyclic amino group-containing, catalysts; for polymerization of α -olefins)

IT 84-74-2, Dibutyl phthalate 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum, uses 115-20-8, 2,2,2-Trichloroethanol 7550-45-0, Titanium tetrachloride, uses 62202-86-2, Butylethylmagnesium 155958-83-1 155958-84-2 155958-85-3 159328-46-8

(catalysts; for polymerization of α -olefins)

L63 ANSWER 33 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:701606 HCAPLUS

DOCUMENT NUMBER: 121:301606

TITLE: Catalysts for polymerization of α -olefins

INVENTOR(S): Kanazawa, Seizaburo; Ishihara, Takeshi; Ookura, Masatoshi; Imanishi, Kunihiko; Ueki, Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**
 LANGUAGE: **Japanese**
 FAMILY ACC. NUM. COUNT: **1**
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06179710	A2	19940628	JP 1992-331458	1992 1211

PRIORITY APPLN. INFO.: <-- JP 1992-331458
 1992
 1211

OTHER SOURCE(S): MARPAT 121:301606

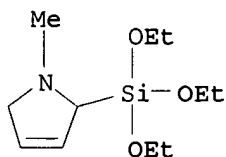
AB The catalysts suitable for manufacture of rigid polyolefins are manufactured by contacting olefins with (A) solid components containing Mg, Ti, halo compds., and electron donors, (B) organic Al compds., and (C) $R_1xR_2ySi(OR_3)z$ (R_1 = N-containing heterocyclic group; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; R_4 = C3-10 hydrocarbyl; R_5 , R_6 = C1-10 hydrocarbyl; $x = 1, 2$; $y = 0, 1$; $z = 2, 3$; $x + y + z = 4$). Thus, propylene was prepolymd. in the presence of a solid component containing $BuMgCl$, Cl_3CCH_2OH , $TiCl_4$, and di-Bu phthalate, Et_3Al , and (2,3,4-trimethyl-3-azacyclopentyl)trimethoxysilane to give a catalyst, which was used to **polymerize** propylene to give a polymer with yield 39.7 kg/g-solid catalyst-h.

IT 155958-85-3

(catalysts for **polymerization** of α -olefins)

RN 155958-85-3 HCAPLUS

CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



IC ICM C08F004-658

CC 35-3 (Chemistry of Synthetic High Polymers)
 Section cross-reference(s): 67

ST catalyst **polymn** olefin heterocyclic alkoxyasilane;
 aluminum magnesium titanium catalyst polyolefin

IT **Polymerization** catalysts

(catalysts for **polymerization** of α -olefins)

IT Silanes

(alkoxy, heterocyclic; catalysts for **polymerization** of α -olefins)

IT Alkenes, preparation

(α -, polymers, catalysts for **polymerization** of α -olefins)

IT 155958-84-2

(catalysts for **polymerization** of α -olefins)

IT 84-74-2, Dibutyl phthalate 97-93-8, Triethylaluminum, uses

100-99-2, Triisobutylaluminum, uses 115-20-8,
 2,2,2-Trichloroethanol 693-04-9, Butylmagnesium chloride
 7550-45-0, Titanium tetrachloride, uses 155958-83-1
 155958-85-3 159328-46-8

(catalysts for polymerization of α -olefins)

IT 9003-07-0P, Polypropylene
 (catalysts for polymerization of α -olefins)

L63 ANSWER 34 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:701594 HCAPLUS

DOCUMENT NUMBER: 121:301594

TITLE: Stereospecific α -olefin
 polymerization catalysts

INVENTOR(S): Ueki, Satoshi; Aoki, Tomoko; Imanishi,
 Kunihiro; Ishihara, Takeshi; Taki, Noryuki;
 Saito, Hiroo

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06145234	A2	19940524	JP 1991-247586	1991 0926
JP 3132680	B2	20010205	JP 1991-247586	1991 0926

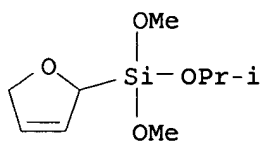
OTHER SOURCE(S): MARPAT 121:301594

AB The title catalysts comprise (A) a solid component containing Mg, Ti, halogen, and electron donor, (B) organometallic compds. and (C) organosilicon compds. R1aR2bSi(OR3)c (R1 = O- or S-containing cyclic residue; R2 = C1-10 hydrocarbyl, R4O, R5Si, R6SiO; R3 = Me, Et; a = 1, 2; b = 0, 1; c = 2, 3; a + b + c = 4; R4 = C3-10 hydrocarbyl; R5, R6 = C1-10 hydrocarbyl). A component was prepared from Mg, Bu2O, BuCl, BuMgCl, Cl3CCH2OH, TiCl4, and di-Bu phthalate and used together with Et3Al and bis(3-tetrahydrofuryl)dimethoxysilane for polymerization of propylene with catalyst efficiency 27.3 kg polymer/g-catalyst component A and heptane-insol. content 97.4%.

IT 158069-58-0
 (stereospecific α -olefin polymerization catalysts)

RN 158069-58-0 HCAPLUS

CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethoxy) - (9CI)
 (CA INDEX NAME)



IC ICM C08F010-00
ICS C08F004-658
CC 35-3 (Chemistry of Synthetic High Polymers)
ST magnesium catalyst olefin **polymn**; titanium catalyst
olefin **polymn**; electron donor catalyst olefin
polymn; silane catalyst olefin **polymn**;
polypropylene manuf catalyst
IT **Polymerization** catalysts
(stereospecific α -olefin **polymerization** catalysts)
IT Silanes
(stereospecific α -olefin **polymerization** catalysts)
IT Alkenes, preparation
(polymers, stereospecific α -olefin **polymerization**
catalysts)
IT 84-74-2, Dibutyl phthalate 97-93-8, Triethylaluminum, uses
109-69-3, Butyl chloride 115-20-8, 2,2,2-Trichloroethanol
142-96-1, Butyl ether 693-04-9, Butylmagnesium chloride
7439-95-4, Magnesium, uses 7550-45-0, Titanium tetrachloride,
uses 158069-53-5 158069-54-6 158069-55-7 158069-56-8
158069-57-9 **158069-58-0** 159412-70-1
(stereospecific α -olefin **polymerization** catalysts)
IT 9003-07-0P, Polypropylene
(stereospecific α -olefin **polymerization** catalysts)

L63 ANSWER 35 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:606267 HCAPLUS

DOCUMENT NUMBER: 121:206267

TITLE: Alkoxysilane-containing **polymerization**
catalysts for α -olefins

INVENTOR(S): Usui, Myuki; Imanishi, Kunihiko; Ishihara,
Takeshi; Ueki, Satoshi

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: **Patent**

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

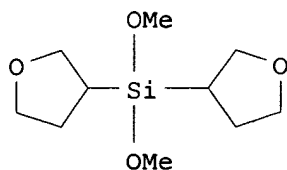
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 06116327	A2	19940426	JP 1992-263476	1992 1001
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PRIORITY APPLN. INFO.:			JP 1992-263476	1992 1001
			<--	

OTHER SOURCE(S): MARPAT 121:206267

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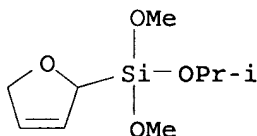
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AB The catalysts contain (A) activated TiCl_3 , (B) organometallic compds., and (C) alkoxy silane $\text{R}_1\text{xR}_2\text{ySi(OR}_3\text{)z}$ (R_1 = monovalent cyclic group with ether or thioether structure; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si , R_6SiO ; R_3 = Me, Et; $\text{x} = 1, 2$; $\text{y} = 0, 1$; $\text{z} = 2, 3$; $\text{x} + \text{y} + \text{z} = 4$; R_4 = C3-10 hydrocarbyl; R_5, R_6 = C1-10 hydrocarbyl). Propylene was **polymerized** by using a catalyst containing (A) a component consisting of Cl_3CCCl_3 and active TiCl_3 made by reducing TiCl_4 with Et_2AlCl and EtAlCl_2 , (B) Et_2AlCl , and (C) silane I. Polypropylene was produced at 6.0 kg/g TiCl_3 component and had crystalline polymer content (boiling heptane-insol.) 98.1%.

IT **158069-58-0**
(alkoxy silane-containing **polymerization** catalysts for α -olefins)

RN 158069-58-0 HCAPLUS

CN Silane, (2,5-dihydro-2-furanyl)dimethoxy(1-methylethoxy) - (9CI)
(CA INDEX NAME)



IC ICM C08F010-00
ICS C08F004-646

CC 35-3 (Chemistry of Synthetic High Polymers)

ST alkoxy silane contg **polymn** catalyst; olefin alpha **polymn** catalyst

IT Silanes
(alkoxy, alkoxy silane-containing **polymerization** catalysts for α -olefins)

IT **Polymerization** catalysts
(modified Ziegler-Natta, alkoxy silane-containing; alkoxy silane-containing **polymerization** catalysts for α -olefins)

IT 96-10-6, Diethylaluminum chloride, uses 97-93-8, Triethylaluminum, uses 158069-53-5 158069-54-6 158069-55-7 158069-56-8 158069-57-9 **158069-58-0**
(alkoxy silane-containing **polymerization** catalysts for α -olefins)

IT 7705-07-9P, Titanium trichloride, preparation
(alkoxy silane-containing **polymerization** catalysts for α -olefins)

IT 25085-53-4P, Polypropylene, isotactic
(alkoxy silane-containing **polymerization** catalysts for α -olefins)

L63 ANSWER 36 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:436448 HCAPLUS

DOCUMENT NUMBER: 121:36448

TITLE: Catalysts for polymerization of α -olefins

INVENTOR(S): Ueki, Satoshi; Aoki, Tomoko; Imanishi, Kunihiro; Ishihara, Takeshi; Taki, Noryuki; Saito, Hiroo

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06025337	A2	19940201	JP 1991-263639	1991 1011

PRIORITY APPLN. INFO.:

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JP 1991-263639

1991
1011

OTHER SOURCE(S): MARPAT 121:36448

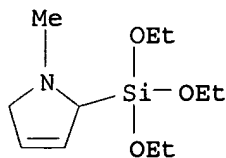
AB Title catalysts to give poly(α -olefins) with high stereoregularity, are composed of (A) solid catalyst components containing metal oxides, Mg, Ti, halogens, and electron donors, (B) organometallic compds., and (C) organic Si compds. of $R_1xR_2ySi(OR_3)z$ (R_1 = N-containing heterocyclic substituent; R_2 = C1-10 hydrocarbyl, R4O, R5Si, R6SiO; R_3 = Me, Et; R_4 = C3-10 hydrocarbyl; R5-6 = C1-10 hydrocarbyl; $x = 1, 2$; $yr = 0, 1$; $z = 2, 3$; $x + y + z = 4$). Thus, 1 L liquid propylene was polymerized at 70° for 1 h in the presence of solid catalyst [prepared from G 952, MgEtBu, Si(OEt)₄, 2,2,2-trichloroethanol, TiCl₄, and di-n-Bu phthalate; Ti content 3.1%], Et₃Al, 2,3,4-trimethyl-3-azacyclopentyltrimethoxysilane, and H in an autoclave to give a polymer showing polymerization activity 10.2 kg/g-solid catalyst and heptane-insol. matter 96.5%.

IT 155958-85-3

(polymerization catalysts, for α -olefins)

RN 155958-85-3 HCAPLUS

CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



IC ICM C08F010-00
ICS C08F004-658

CC 35-4 (Chemistry of Synthetic High Polymers)
 ST olefin **polymn** catalyst modified Ziegler; org silicon
 compd **polymn** catalyst; titanium magnesium halogen
polymn catalyst; electron donor **polymn** catalyst;
 metal oxide **polymn** catalyst
 IT Organometallic compounds
 (catalysts, for α -olefin **polymerization**)
 IT **Polymerization** catalysts
 (stereospecific, metal oxide-magnesium-titanium-halogen-
 electron donor solids and organometallic compds. and organic
 silicon compds., for α -olefins)
 IT Alkenes, preparation
 (α -, polymers, preparation of, **polymerization** catalysts
 for, metal oxide-magnesium-titanium-halogen-electron donor
 solids and organometallic compds. and organic silicon compds. as)
 IT 78-10-4, Tetraethoxysilane 84-74-2 115-20-8,
 2,2,2-Trichloroethanol 7550-45-0, Titanium tetrachloride, uses
 7631-86-9, Silica, uses 62202-86-2
 (catalysts containing, for **polymerization** of α -olefins)
 IT 97-93-8, Triethylaluminum, uses 155958-83-1 155958-84-2
 155958-85-3
 (polymerization catalysts, for α -olefins)
 IT 25085-53-4P
 (preparation of, **polymerization** catalysts for)

L63 ANSWER 37 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:436447 HCAPLUS

DOCUMENT NUMBER: 121:36447

TITLE: Catalysts for **polymerization** of
 α -olefins

INVENTOR(S): Ueki, Satoshi; Aoki, Tomoko; Imanishi,
 Kunihiro; Ishihara, Takeshi; Taki, Noriyuki;
 Saito, Hiroo

PATENT ASSIGNEE(S): Tonen Corp, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06025336	A2	19940201	JP 1991-263638	1991 1011

PRIORITY APPLN. INFO.: JP 1991-263638

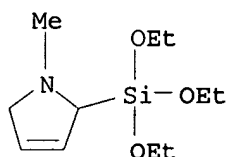
1991
1011

OTHER SOURCE(S): MARPAT 121:36447

AB Title catalysts to give poly(α -olefins) with high
 stereoregularity, are composed of (A) solid catalyst components
 containing Mg, Ti, halogens, and electron donors, (B) organometallic
 compds., and (C) organic Si compds. of $R_1xR_2ySi(OR_3)z$ (R_1 = N-containing
 heterocyclic substituent; R_2 = C1-10 hydrocarbyl, R_4O , R_5Si ,
 R_6SiO ; R_3 = Me, Et; R_4 = C3-10 hydrocarbyl; R_5-6 = C1-10
 hydrocarbyl; $x = 1, 2$; $yr = 0, 1$; $z = 2, 3$; $x + y + z = 4$). Thus,

1 L liquid propylene was **polymerized** at 70° for 1 h in the presence of solid catalyst [prepared from Mg, n-Bu₂O, n-BuMgCl, n-BuCl, HC(OEt)₃, 2,2,2-trichloroethanol, TiCl₄, and di-n-Bu phthalate], Et₃Al, 2,3,4-trimethyl-3-azacyclopentyltrimethoxysilane, and H in an autoclave to give a polymer showing **polymn** activity 15.1 kg/g-solid catalyst and heptane-insol. matter 97.4%.

IT 155958-85-3
(polymerization catalysts, for α-olefins)
RN 155958-85-3 HCAPLUS
CN 1H-Pyrrole, 2,5-dihydro-1-methyl-2-(triethoxysilyl)- (9CI) (CA INDEX NAME)



IC ICM C08F010-00
ICS C08F004-654
CC 35-4 (Chemistry of Synthetic High Polymers)
ST olefin **polymn** catalyst organometallic compd; org silicon compd **polymn** catalyst; titanium magnesium halogen **polymn** catalyst; electron donor **polymn** catalyst
IT Organometallic compounds
(catalysts, for α-olefin **polymerization**)
IT **Polymerization** catalysts
(stereospecific, magnesium-titanium-halogen-electron donor solids and organometallic compds. and organic silicon compds., for α-olefins)
IT Alkenes, preparation
(α-, polymers, preparation of, **polymerization** catalysts for, magnesium-titanium-halogen-electron donor solids and organometallic compds. and organic silicon compds. as)
IT 84-74-2 109-69-3, n-Butyl chloride 115-20-8, 2,2,2-Trichloroethanol 122-51-0, Triethoxymethane 142-96-1, n-Butyl ether 693-04-9, n-Butylmagnesium chloride 7439-95-4, Magnesium, uses 7550-45-0, Titanium tetrachloride, uses (catalysts containing, for **polymerization** of α-olefins)
IT 97-93-8, Triethylaluminum, uses 155958-83-1 155958-84-2 155958-85-3
(polymerization catalysts, for α-olefins)
IT 25085-53-4P
(preparation of, **polymerization** catalysts for)

L63 ANSWER 38 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:308504 HCAPLUS
DOCUMENT NUMBER: 120:308504
TITLE: Conductive polymer oxidation catalyst and oxidation method
INVENTOR(S): Ooshiro, Yoshiki; Hirao, Shunichi
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05253489	A2	19931005	JP 1992-53867	1992 0312

PRIORITY APPLN. INFO.:

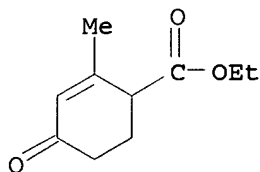
<--
 JP 1992-53867
 1992
 0312

AB A catalyst for oxidizing an organic compound having ≥ 1 H comprises a conductive polymer. A method for oxidizing an organic compound having ≥ 1 H involves oxidizing in the presence of the above catalyst and an optional transition metal.

IT 487-51-4
 (oxidation of, catalyst for)

RN 487-51-4 HCAPLUS

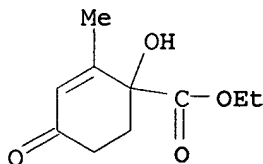
CN 2-Cyclohexene-1-carboxylic acid, 2-methyl-4-oxo-, ethyl ester
 (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 155085-77-1P
 (preparation of, oxidation catalyst for)

RN 155085-77-1 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 1-hydroxy-2-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



IC ICM B01J031-06
 ICS C07B033-00; C07C045-38; C07C047-232; C07C069-757; C07C251-08;
 C07C251-18; C07C251-24

ICA C07B061-00

CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

Section cross-reference(s): 23, 24, 38, 76

IT Electric conductors, polymeric
 (oxidation catalysts)

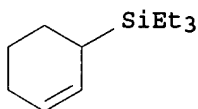
IT 100-46-9, Benzylamine, reactions 104-54-1 487-51-4
 2835-06-5, 2-Phenylglycine

(oxidation of, catalyst for)
 IT 104-55-2P 780-25-6P, N-Benzylidene benzylamine
 155085-77-1P
 (preparation of, oxidation catalyst for)

L63 ANSWER 39 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1994:107946 HCAPLUS
 DOCUMENT NUMBER: 120:107946
 TITLE: New routes to phenylsilicones
 AUTHOR(S): Stein, Judith; Lettko, Kevin X.; King, Joseph
 A.; Colborn, Robert E.
 CORPORATE SOURCE: Phys. Chem. Lab., GE Res. Dev., Schenectady,
 NY, 12301, USA
 SOURCE: Journal of Applied Polymer Science (1994),
 51(5), 815-22
 CODEN: JAPNAB; ISSN: 0021-8995
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Two alternative nonhalogen routes for the synthesis of Ph
 siloxanes are explored. In the first method, 2,3-
 dimethylbutadiene is reacted with divinyltetramethyldisiloxane via
 a Diels-Alder reaction. The product can then be aromatized. In
 the second method, cyclohexadiene undergoes hydrosilylation and
 the resultant product can be aromatized using Pd/C with PhNO₂ as
 an electron acceptor. Ph silicones can be prepared in a single step
 in which a silicon hydride fluid and cyclohexadiene are refluxed
 in the presence of Pt/C and PhNO₂.

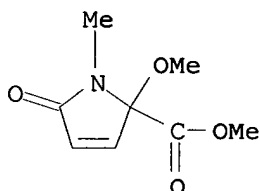
IT 92992-63-7P
 (preparation and acid hydrolysis of)
 RN 92992-63-7 HCAPLUS
 CN Silane, 2-cyclohexen-1-yltriethyl- (9CI) (CA INDEX NAME)



CC 35-7 (Chemistry of Synthetic High Polymers)
 IT **Polymerization**
 (Diels-Alder, Ph silicones prepared from)
 IT **Polymerization**
 (hydrosilylation, Ph silicones prepared from)
 IT 92992-63-7P
 (preparation and acid hydrolysis of)
 IT 56-33-7P
 (preparation and **polymerization** of, with
 octamethylcyclotetrasiloxane)

L63 ANSWER 40 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1990:76851 HCAPLUS
 DOCUMENT NUMBER: 112:76851
 TITLE: Electrochemical oxidation of pyrrole
 derivatives in alcoholic medium
 AUTHOR(S): Tedjar, Farouk; Ymmel, Salah; Janda, Miroslav;
 Duchek, Petr; Holy, Petr; Stibor, Ivan
 CORPORATE SOURCE: Dep. Electrochem., Setif Univ., Setif, Algeria
 SOURCE: Collection of Czechoslovak Chemical
 Communications (1989), 54(5), 1299-305

CODEN: CCCCCA; ISSN: 0010-0765
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 112:76851
 AB Electrochem. oxidation of pyrrole, 1-methylpyrrole (I), 1,2,5-trimethylpyrrole (II), Me 1-methyl-2-pyrrolecarboxylate (III), and di-Et 3,5-dimethyl-2,4-pyrroledicarboxylate (IV) was studied. Electrochem. methoxylation of pyrrole gave poly(pyrrole); low-mol.-weight oxidation products were obtained from N-substituted pyrrole derivs. Electrooxidn. of I in MeOH gave 5,5-dimethoxy-1-methyl-3-pyrrolin-2-one or 1-methyl-2,2,5,5-tetramethoxy-3-pyrroline, their ratio depending on the H₂O content in the alc. used. Oxidation of III affords the analogous 5-carbomethoxy-5-methoxy-1-methyl-3-pyrrolin-2-one; oxidation of II and IV leads to products of substitution at the Me groups.
 IT 125101-10-2P
 (preparation of)
 RN 125101-10-2 HCAPLUS
 CN 1H-Pyrrole-2-carboxylic acid, 2,5-dihydro-2-methoxy-1-methyl-5-oxo-, methyl ester (9CI) (CA INDEX NAME)



CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 35, 72
 ST electrochem oxidn pyrrole; electropolymer pyrrole; **polymn**
 electrochem pyrrole
 IT **Polymerization**
 (electrochem., of pyrrole)
 IT 9002-86-2DP, reaction products with pyrrole 13131-30-1P
 13131-31-2P 77632-07-6P 125101-09-9P 125101-10-2P
 125166-23-6P
 (preparation of)
 L63 ANSWER 41 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1989:554515 HCAPLUS
 DOCUMENT NUMBER: 111:154515
 TITLE: Manufacture of di(meth)acryloyloxyethyl esters
 of tetracarboxylic acids
 INVENTOR(S): Kitamura, Taku; Takahashi, Katsuji
 PATENT ASSIGNEE(S): Dainippon Ink and Chemicals, Inc., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: **Patent**
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63255249	A2	19881021	JP 1987-89777	

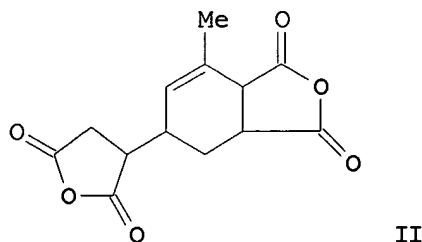
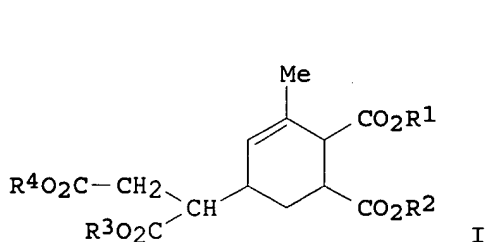
1987
0414

PRIORITY APPLN. INFO.:

<--
JP 1987-897771987
0414OTHER SOURCE(S):
GI

MARPAT 111:154515

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AB UV-curable title compds. I (R1-4 = H, CH₂CH₂O₂CCH:CH₂, CH₂CH₂O₂CCMe:CH₂ excluding R1 = R2 = R3 = R4) are prepared by treating the dianhydride II with β-hydroxyethyl (meth)acrylate in the presence of a catalyst and a **polymn** . inhibitor. Thus, 264 g II was added in 5 portions over 1 h to a mixture of β-hydroxyethyl acrylate 232, dimethylaminopyridine 0.5, hydroquinone 4.0, and toluene 340 g at 60° and heated at 60° for 2 h and then at 80° for 2 h to give a mixture of I (two of R1-4 are CH₂CH₂O₂CCH:CH₂ while the other two are H).

IT 121150-51-4P 121150-52-5P
(preparation of, UV-curable)

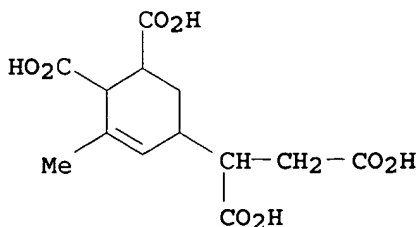
RN 121150-51-4 HCAPLUS

CN 3-Cyclohexene-1,2-dicarboxylic acid, 5-(1,2-dicarboxyethyl)-3-methyl-, bis[2-[(1-oxo-2-propenyl)oxy]ethyl] ester (9CI) (CA INDEX NAME)

CM 1

CRN 121150-50-3

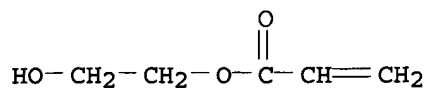
CMF C13 H16 O8



CM 2

CRN 818-61-1

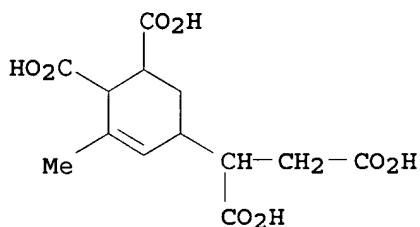
CMF C5 H8 O3



RN 121150-52-5 HCAPLUS
 CN 3-Cyclohexene-1,2-dicarboxylic acid, 5-(1,2-dicarboxyethyl)-3-methyl-, bis[2-[(1-methyl-1-oxo-2-propenyl)oxy]ethyl] ester (9CI)
 (CA INDEX NAME)

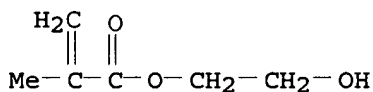
CM 1

CRN 121150-50-3
 CMF C13 H16 O8



CM 2

CRN 868-77-9
 CMF C6 H10 O3



IC ICM C07C069-75
 ICS B01J031-02; C07C067-10
 CC 35-2 (Chemistry of Synthetic High Polymers)
 IT **Polymerization inhibitors**
 (in ring-opening half-esterification of
 (dioxotetrahydrofuran-2-yl)methylcyclohexenedicarboxylic acid
 anhydride with hydroxyethyl (meth)acrylate)
 IT 123-31-9, Hydroquinone, uses and miscellaneous 150-76-5,
 Hydroquinone monomethyl ether
 (polymerization inhibitor, in esterification of
 (dioxotetrahydrofuran-2-yl)methylcyclohexenedicarboxylic acid
 anhydride with hydroxyethyl (meth)acrylate)
 IT 121150-51-4P 121150-52-5P
 (preparation of, UV-curable)

L63 ANSWER 42 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1988:76290 HCAPLUS
 DOCUMENT NUMBER: 108:76290
 TITLE: Synthesis and characterization of iron(III)

chelating analogs of siderophores on organic solid supports

AUTHOR(S): Crumbliss, A. L.; Garrison, J. M.; Bock, C. R.; Schaaf, A.; Bonaventura, C. J.; Bonaventura, J.

CORPORATE SOURCE: Dep. Chem., Duke Univ., Durham, NC, 27706, USA

SOURCE: Inorganica Chimica Acta (1987), 133(2), 281-7
CODEN: ICHAA3; ISSN: 0020-1693

DOCUMENT TYPE: Journal

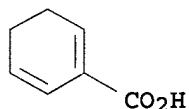
LANGUAGE: English

AB A series of iron(III)-selective chelating resins have been modeled after the structural features of the naturally occurring siderophore compds. with hydroxamate, catecholate and salicylate iron binding groups. Amberlite IRC-50 was derivatized via an acid chloride intermediate to produce poly(hydroxamic acid) and polysalicylate chelating resins with enhanced iron(III) binding capacity. As an alternative synthetic approach, a poly(amidoxime) (PAO) chelating resin was synthesized from 846:21:184:25 acrylonitrile-divinylbenzene-Et acrylate-styrene copolymer. Comparison between the 2 synthetic approaches showed that PAO bound a greater amount of iron(III) at flow-through column conditions, while a IRC-50 poly(hydroxamic acid) derivative exhibited a greater iron(III) binding capacity under batch equilibration conditions.

IT 40002-23-1DP, 3,4-Dihydrobenzoic acid, reaction products with amberlite IRC 50 derivs.
(chelating resins, preparation of, for iron, as siderophore analog)

RN 40002-23-1 HCAPLUS

CN 1,5-Cyclohexadiene-1-carboxylic acid (6CI, 9CI) (CA INDEX NAME)



CC 37-3 (Plastics Manufacture and Processing)
Section cross-reference(s): 38

IT Amidoximes
Hydroxamic acids
(polymeric, as chelating resins for iron)

IT 9002-29-3DP, Amberlite IRC 50, derivs. 40002-23-1DP, 3,4-Dihydrobenzoic acid, reaction products with amberlite IRC 50 derivs. 70120-40-0DP, reaction products with amberlite IRC 50 derivs. 112782-83-9DP, hydroxamic acid and amidoxime derivs.
(chelating resins, preparation of, for iron, as siderophore analog)

L63 ANSWER 43 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:540488 HCAPLUS

DOCUMENT NUMBER: 99:140488

TITLE: Electron donor-acceptor monomers and polymers. Synthesis and polymerization of 7,8-dialkoxycarbonyl-7,8-dicyanoquinodimethanes

AUTHOR(S): Mulvaney, J. E.; Hall, H. K., Jr.; Cramer, R. J.

CORPORATE SOURCE: Dep. Chem., Univ. Arizona, Tucson, AZ, 85721, USA

SOURCE: Proc. IUPAC, I. U. P. A. C., Macromol. Symp.,

28th (1982), 158. Int. Union Pure Appl.
Chem.: Oxford, UK.
CODEN: 50DXAF

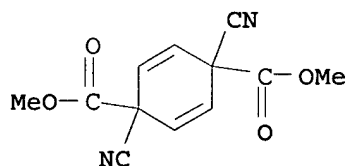
DOCUMENT TYPE:

Conference

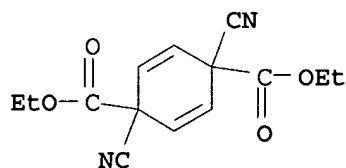
LANGUAGE:

English

- AB 7,8-Di(methoxycarbonyl)-7,8-dicyanoquinodimethane (I) [87340-68-9] and 7,8-di(ethoxycarbonyl)-7,8-dicyanoquinodimethane (II) [87340-69-0] **polymd** . instantaneously upon dissolving in MeCN, DMSO, DMF, and sulfolane, and **polymerized** within 1h in CHCl₃ in the absence of catalyst. **Polymerization** of II gave soluble polymers of moderate mol. weight, which formed transparent, flexible films when cast from CHCl₃ solns. High conversions to an insol. polymer were observed with I. Attempted copolymns. of I and II with nucleophilic olefins gave only homopolymers of I and II. I and II were prepared by treating p-xylylenedicyanide [622-75-3] with NaH and dialkyl carbonate to give the α,α' -bis(alkoxycarbonyl)-p-xylylenedicyanide, which was oxidized to the corresponding quinodimethane. I had an electron-accepting ability (voltammetric reduction potential-0.65 V) between TCNQ and tetra(methoxycarbonyl)quinodimethane.
- IT 87340-68-9P
(preparation and electron-acceptor properties and **polymerization** of)
- RN 87340-68-9 HCAPLUS
- CN 2,5-Cyclohexadiene-1,4-dicarboxylic acid, 1,4-dicyano-, dimethyl ester (9CI) (CA INDEX NAME)



- IT 87340-69-0P
(preparation and **polymerization** of)
- RN 87340-69-0 HCAPLUS
- CN 2,5-Cyclohexadiene-1,4-dicarboxylic acid, 1,4-dicyano-, diethyl ester (9CI) (CA INDEX NAME)



- CC 35-4 (Chemistry of Synthetic High Polymers)
- ST methoxycarbonyldicyanoquinodimethane prepn **polymn**;
ethoxycarbonyldicyanoquinodimethane prepn **polymn**;
dicyanoquinodimethane dialkoxycarbonyl prepn **polymn**;
quinodimethane dicyano dialkoxycarbonyl prepn **polymn**;
polymn dialkoxycarbonyldicyanoquinodimethane; electron
acceptor dialkoxycarbonyldicyanoquinodimethane
- IT Electron acceptors

(bis(alkoxycarbonyl)dicyanoquinodimethanes, **polymerization** and properties of)
 IT **Polymerization**
 (of bis(methoxycarbonyl)dicyanoquinodimethane)
 IT **87340-68-9P**
 (preparation and electron-acceptor properties and **polymerization** of)
 IT **87340-69-0P**
 (preparation and **polymerization** of)

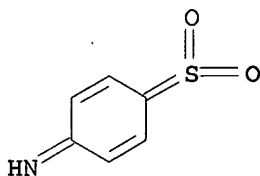
L63 ANSWER 44 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1981:516040 HCAPLUS
 DOCUMENT NUMBER: 95:116040
 TITLE: Synthesis of poly(p-benzenesulfonamide). Part III. Solution **polymerization**
 AUTHOR(S): Contreras, Jordi; Jones, J. Idris
 CORPORATE SOURCE: Dep. Non Metall. Mater., Brunel Univ., Uxbridge, UB8 3PH, UK
 SOURCE: British Polymer Journal (1980), 12(4), 205-11
 CODEN: BPOJAB; ISSN: 0007-1641
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Poly(p-benzenesulfonamide) was prepared by the solution **polymn** . of p-OSNC6H4SO2Cl (I) [46204-38-0], p-H2NC6H4SO2Cl (II) [24939-24-0], and p-ClSO2C6H4NH2.HCL (III) [78798-60-4] at low temps. in the presence of a base. In the case of II and III, 4-iminocyclohexadiene sulfene [78810-64-7] was formed as an intermediate. On addition of 1 equiv H2O in the **polymn** . of I, II was formed and **polymerization** ensued via the same intermediate. Similarly, poly(N-methyl-p-benzenesulfonamide) was formed by solution **polymerization** of p-ClSO2C6H4NHMe.HCl [78798-61-5]. **Polymerization** of crystalline III was also effected in the solid state in a nonsolvent. Certain amide solvents were unsuitable for the **polymerization** of III. DMF [68-12-2] and N-methylpyrrolidone [872-50-4] condensed with III and in the case of (Me2N)2CO, some **polymerization** occurred but the yield and mol. weight of the polymer were low.

IT **78810-64-7P**
 (formation of, in solution **polymerization** of aniline sulfochloride and its derivs.)

RN 78810-64-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-thione, 4-imino-, S,S-dioxide (9CI) (CA INDEX NAME)



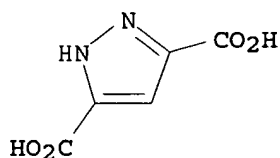
CC 35-3 (Synthetic High **Polymers**)
 ST aniline sulfochloride soln **polymn**; hydrochloride aniline sulfochloride **polymn**; sulfinylaniline sulfochloride soln **polymn**; methylaniline sulfochloride hydrochloride **polymn**; iminocyclohexadiene sulfene formation
 IT **Polymerization**
 (solution, of aniline sulfochloride, aniline sulfochloride

hydrochloride and sulfinylaniline sulfochloride, mechanism of)
 IT 78810-64-7P
 (formation of, in solution **polymerization** of aniline
 sulfochloride and its derivs.)
 IT 24939-24-0 46204-38-0 78798-60-4 78798-61-5
 (**polymerization** of, solution, mechanism of)

L63 ANSWER 45 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1980:495694 HCAPLUS
 DOCUMENT NUMBER: 93:95694
 TITLE: New polyimidazolyl and pyrazolyl esters
 AUTHOR(S): Dumitriu, S.; Dumitriu, Maria; Blascu, V.
 CORPORATE SOURCE: Dep. Org. Macromol. Chem., Polytech. Inst.
 Jassy, Iasi, 6600, Rom.
 SOURCE: Polymer Bulletin (Berlin, Germany) (1980),
 2(8), 565-70
 CODEN: POBUDR; ISSN: 0170-0839
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The title esters were synthesized by polycondensation of the acid
 chlorides of imidazolyl and pyrazolyl dicarboxylic acids with
 ethylene glycol, pentamethylene glycol, or glycerol. Macromol.
 cyclic esters were found in the polyesters prepared with ethylene
 glycol; linear structures were obtained using pentamethylene
 glycol and glycerol. The polyesters exhibited good thermal
 stability, were soluble in strong acids, and were partially soluble in
 DMF, hot pyridine, and N-methylpyrrolidone.

IT 3112-31-0P
 (preparation and reaction of, with thionyl chloride)
 RN 3112-31-0 HCAPLUS
 CN 1H-Pyrazole-3,5-dicarboxylic acid (9CI) (CA INDEX NAME)



CC 35-3 (Synthetic High Polymers)
 IT **Polymerization**
 (condensation, of imidazolyl- and pyrazolyl dicarboxylic acid
 chlorides with glycols)
 IT 74669-18-4P
 (formation of, in **polymerization** of ethylene glycol with
 imidazolyl dicarboxylic acid dichloride)
 IT 74669-17-3P
 (formation of, in **polymerization** of ethylene glycol with
 pyrazolyl dicarboxylic acid dichloride)
 IT 35344-96-8P 59399-36-9P
 (preparation and **polymerization** of, with glycols)
 IT 570-22-9P 3112-31-0P
 (preparation and reaction of, with thionyl chloride)

L63 ANSWER 46 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1980:426881 HCAPLUS
 DOCUMENT NUMBER: 93:26881
 TITLE: Conjugative effect of the pyridazinone ring on

the copolymerizabilities of substituted pyridazinones

AUTHOR(S): Eda, Tsunehito; Matsubara, Yoshio; Yoshihara, Masakuni; Maeshima, Toshihisa

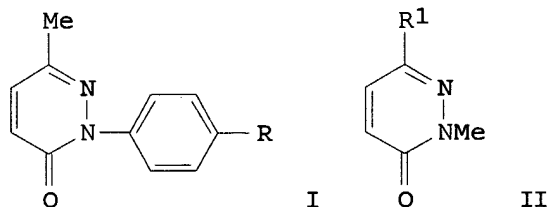
CORPORATE SOURCE: Fac. Sci. Eng., Kinki Univ., Higashi-Osaka, 577, Japan

SOURCE: Journal of Macromolecular Science, Chemistry (1980), A14(5), 771-8
CODEN: JMCHBD; ISSN: 0022-233X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



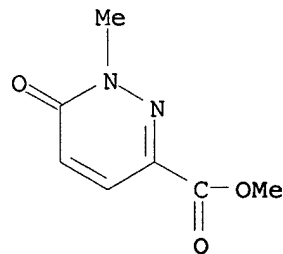
AB Free-radical polymerization of pyridazinones I (R = Me, H, Cl, MeO) and II (R1 = H, Cl, CO2Me) with styrene [100-42-5] or acrylonitrile [107-13-1] was carried out in DMF at 60° and values of Hammett's σ and ρ , reactivity ratios, and Q-e values were determined. In the case of II and styrene the reactivities were nicely correlated with Otsu's equation, suggesting that the growing radicals of II are stabilized by the resonance contributions of the substituents of II at their transition states. All observations were discussed in terms of the conjugative effect of the pyridazinone ring.

IT 74173-58-3P

(preparation and polymerization of, with acrylonitrile or styrene, conjugative effect in)

RN 74173-58-3 HCAPLUS

CN 3-Pyridazinecarboxylic acid, 1,6-dihydro-1-methyl-6-oxo-, methyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 35-4 (Synthetic High Polymers)

ST Hammett substituent const pyridazinone polymn;
pyridazinone deriv polymn styrene acrylonitrile;
reactivity ratio pyridazinone deriv polymn; conjugative
effect pyridazinone copolymn

IT Conjugation

- (in pyridazinones, **polymerization** with acrylonitrile or styrene in relation to)
- IT Q-e value in **polymerization**
Reactivity ratio in **polymerization**
(of pyridazinones with acrylonitrile or styrene)
- IT **Polymerization**
(of pyridazinones with acrylonitrile or styrene, conjugative effect in)
- IT Substituent constant
(Hammett, of pyridazinones, **polymerization** with acrylonitrile and styrene in relation to)
- IT 100-42-5, reactions 107-13-1, reactions
(**polymerization** of, with substituted pyridazinones, conjugative effect on)
- IT 6296-86-2P 10071-38-2P 22687-56-5P 37986-37-1P 38154-50-6P
74173-58-3P 74173-59-4P
(preparation and **polymerization** of, with acrylonitrile or styrene, conjugative effect in)

L63 ANSWER 47 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1979:138249 HCAPLUS

DOCUMENT NUMBER: 90:138249

TITLE: Synthesis and properties of chelate resins with pyrazole-3,4-dicarboxylic acid and 1,2,3-triazole-4,5-dicarboxylic acid as anchor groups

AUTHOR(S): Manecke, Georg; Ruehl, Christian Steffen

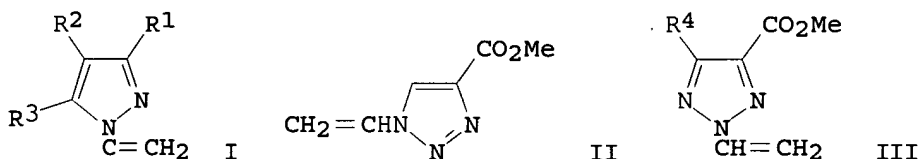
CORPORATE SOURCE: Inst. Org. Chem., Freie Univ. Berlin, Berlin, Fed. Rep. Ger.

SOURCE: Makromolekulare Chemie (1979), 180(1), 103-15
CODEN: MACEAK; ISSN: 0025-116X

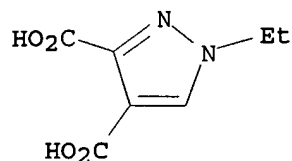
DOCUMENT TYPE: Journal

LANGUAGE: German

GI



- AB I (R1 = H, CO2Et, CO2Me; R2 = H, CO2Me; R3 = H, CO2Et), II [69463-20-3], and III (R4 = H, CO2Me) were prepared by the N-vinylation of the appropriate heterocycle with vinyl acetate [108-05-4] in the presence of Hg acetate and oleum. I (R1 = R2 = CO2Me, R3 = H [69457-68-7] and III (R4 = CO2Me) [69457-72-3] were copolymd. with divinylbenzene to crosslinked products and saponified to CO2H-containing resins. These resins showed a sharp increase in swelling at pH 7-9. The complexation of heavy metals (Cu, Vn, and Mg) by the resins increased on increasing the pH from 1.2 to 5.5.
- IT 52942-75-3P
(preparation and acidity constant of, as chelating resin model compound)
- RN 52942-75-3 HCAPLUS
- CN 1H-Pyrazole-3,4-dicarboxylic acid, 1-ethyl- (9CI) (CA INDEX NAME)

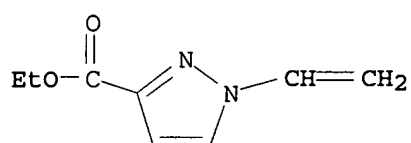


IT 69457-64-3P 69457-68-7P

(preparation and polymerization of)

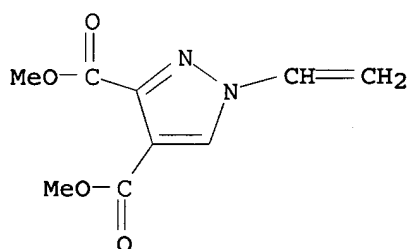
RN 69457-64-3 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 1-ethenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 69457-68-7 HCAPLUS

CN 1H-Pyrazole-3,4-dicarboxylic acid, 1-ethenyl-, dimethyl ester (9CI) (CA INDEX NAME)

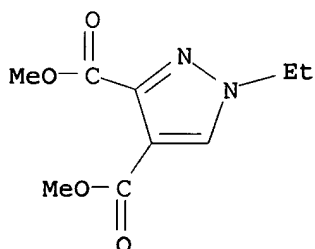


IT 69463-17-8P

(preparation and saponification of)

RN 69463-17-8 HCAPLUS

CN 1H-Pyrazole-3,4-dicarboxylic acid, 1-ethyl-, dimethyl ester (9CI) (CA INDEX NAME)

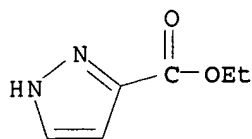


IT 5932-27-4 33090-46-9

(vinylation of)

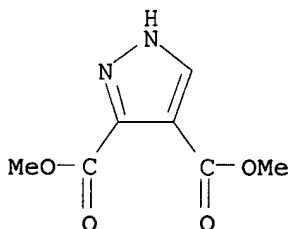
RN 5932-27-4 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, ethyl ester (9CI) (CA INDEX NAME)



RN 33090-46-9 HCAPLUS

CN 1H-Pyrazole-3,4-dicarboxylic acid, dimethyl ester (9CI) (CA INDEX NAME)



CC 35-3 (Synthetic High Polymers)
Section cross-reference(s): 28, 78

IT **Polymerization**
(of vinylpyrazoledicarboxylic and vinyltriazoledicarboxylic acids)

IT **52942-75-3P** 69463-19-0P
(preparation and acidity constant of, as chelating resin model compound)

IT **69457-64-3P** 69457-66-5P **69457-68-7P**
69457-70-1P 69457-72-3P

(preparation and **polymerization** of)

IT 69457-74-5P 69457-75-6P **69463-17-8P** 69463-18-9P
(preparation and saponification of)

IT 707-94-8 4967-77-5 **5932-27-4** **33090-46-9**
(vinylation of)

L63 ANSWER 48 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1977:406392 HCAPLUS

DOCUMENT NUMBER: 87:6392

TITLE: Vinyl monomers based on pyridazone and its derivatives

AUTHOR(S): Mikhant'ev, B. I.; Shatalov, G. V.; Gridchin, S. A.

CORPORATE SOURCE: Voronezh. Gos. Univ., Voronezh, USSR
SOURCE: Izvestiya Vysshikh Uchebnykh Zavedenii,
Khimiya i Khimicheskaya Tekhnologiya (1977),
20(3), 419-22

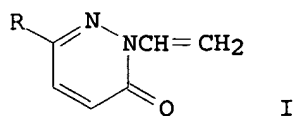
CODEN: IVUKAR; ISSN: 0579-2991

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 87:6392

GI

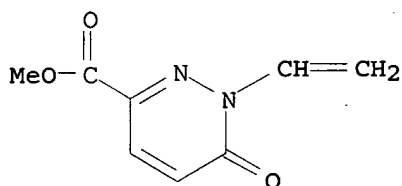


AB Vinylation of 3-pyridazinone [504-30-3] and its 6-substituted derivs. with acetylene [74-86-2] under pressure gave the corresponding compds. I (R = H, Me, Ph, CO₂Me, CO₂Et, CO₂Pr, CO₂Pr-iso, CO₂Bu) in yields ≤60%. Dioxane and THF were used as solvents. The reaction was catalyzed by KOH, CdO, ZnO, and (AcO)₂Cd [543-90-8]. The structure of I was established by elemental anal., mol. weight determination, IR spectroscopy, and chromatog. I were **polymerizable** and some of them had antihypertensive activity.

IT 63001-25-2P 63001-26-3P 63001-27-4P
63001-28-5P 63001-29-6P
(preparation of)

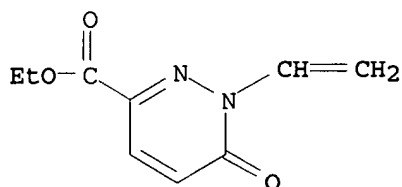
RN 63001-25-2 HCAPLUS

CN 3-Pyridazinecarboxylic acid, 1-ethenyl-1,6-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)



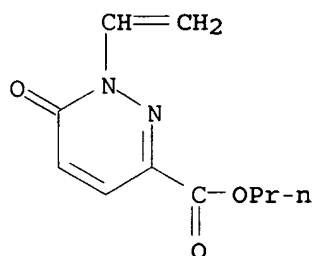
RN 63001-26-3 HCAPLUS

CN 3-Pyridazinecarboxylic acid, 1-ethenyl-1,6-dihydro-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)



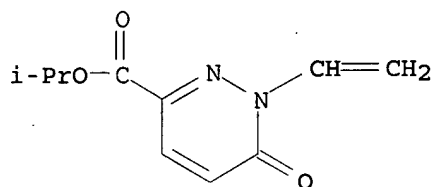
RN 63001-27-4 HCAPLUS

CN 3-Pyridazinecarboxylic acid, 1-ethenyl-1,6-dihydro-6-oxo-, propyl
ester (9CI) (CA INDEX NAME)



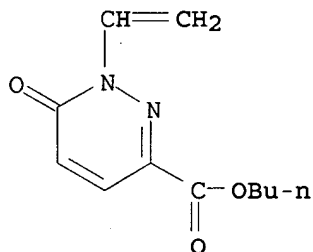
RN 63001-28-5 HCAPLUS

CN 3-Pyridazinecarboxylic acid, 1-ethenyl-1,6-dihydro-6-oxo-,
1-methylethyl ester (9CI) (CA INDEX NAME)



RN 63001-29-6 HCAPLUS

CN 3-Pyridazinecarboxylic acid, 1-ethenyl-1,6-dihydro-6-oxo-, butyl
ester (9CI) (CA INDEX NAME)



CC 35-2 (Synthetic High Polymers)

Section cross-reference(s): 1, 28

ST vinylation pyridazinone; antihypertensive vinylpyridazinone;
vinylpyridazinone polymn antihypertensive activity

IT 50862-92-5P 63001-24-1P 63001-25-2P

63001-26-3P 63001-27-4P 63001-28-5P

63001-29-6P 63001-35-4P

(preparation of)

L63 ANSWER 49 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:44131 HCAPLUS

DOCUMENT NUMBER: 82:44131

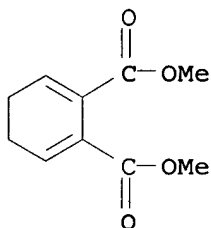
TITLE: Amphoteric ion exchangers. 5

AUTHOR(S): Manecke, Georg; Aurich, Hans P.; Gergs, Peter;
Langisch, Hans

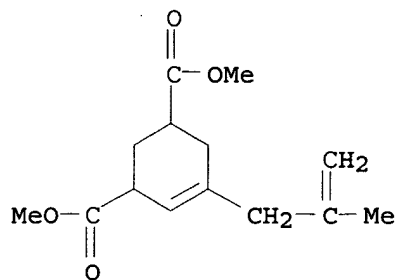
CORPORATE SOURCE: Inst. Org. Chem., Freie Univ. Berlin,
Berlin-Dahlem, Fed. Rep. Ger.

SOURCE: Makromolekulare Chemie (1974), 175(6), 1833-45

CODEN: MACEAK; ISSN: 0025-116X
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Amphoteric ion exchange resins with a homogeneous distribution of exchange groups were prepared by copolymerizing aziridinyl-substituted esters and then hydrolyzing. A typical resin was saponified di-Et 2,4-di(1-aziridinyl)glutarate-di-Et (1-aziridinyl)succinate polymer [53540-62-8], which had base (OH-) binding capacity 8.42 mmole/g, Cu²⁺ binding capacity 3.65 mmole/g at pH 6, and water content in the air-dried zwitterionic form 11.9%. The divalent Cu, Ni, Zn, and Mg ion binding capacity and sp. volume of the resins increased with increasing pH in the ranges 2-6 and 2-9, resp.
IT 53523-27-6
(reaction of, with aziridine)
RN 53523-27-6 HCAPLUS
CN 2,6-Cyclohexadiene-1,2-dicarboxylic acid, dimethyl ester (7CI, 9CI) (CA INDEX NAME)



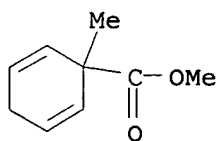
CC 36-3 (Plastics Manufacture and Processing)
IT Polymerization
(of aziridinyl-substituted esters)
IT 53523-27-6 53523-28-7
(reaction of, with aziridine)
L63 ANSWER 50 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:72849 HCAPLUS
DOCUMENT NUMBER: 76:72849
TITLE: Allene cyclooligomerization and polymerization catalyzed by a nickel(0) complex
AUTHOR(S): De Pasquale, Ralph J.
CORPORATE SOURCE: Shell Dev. Co., Emeryville, CA, USA
SOURCE: Journal of Organometallic Chemistry (1971), 32(3), 381-93
CODEN: JORCAI; ISSN: 0022-328X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bis(triphenylphosphine)nickel(0) [33991-60-5] converts allene into a mixture of cyclic trimers, a tetramer, a pentamer, isomeric hexamers, waxes, and polyallene [24979-93-9]. The complex initially formed is (Ph₃P)₂NiC₃H₄. Competitive reactions with ethylene [74-85-1] and Me acrylate [96-33-3] show intervention of subsequent complexes in the formation of linear, monocyclic, and bicyclic products.
IT 35061-83-7P
(preparation of, by allene-Me acrylate cooligomerization)
RN 35061-83-7 HCAPLUS
CN 4-Cyclohexene-1,3-dicarboxylic acid, 5-(2-methyl-2-propenyl)-, dimethyl ester (9CI) (CA INDEX NAME)



CC 35 (Synthetic High Polymers)
 Section cross-reference(s): 24, 29, 23
 IT **Polymerization**
 (mechanism of, of allene)
 IT **Polymerization** catalysts
 (nickel complexes, for allene)
 IT 33991-60-5
 (catalysts, for **polymerization** and cyclooligomerization of
 allene)
 IT 35061-81-5P 35061-82-6P **35061-83-7P**
 (preparation of, by allene-Me acrylate cooligomerization)

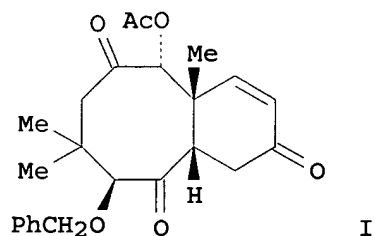
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L62 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2000:433733 HCAPLUS
 DOCUMENT NUMBER: 134:56336
 TITLE: Theoretical studies of the stability of
 8a-alkyl-1,2,3,4,6,8a-hexahydronaphthalen-1-
 ones using semiempirical methods
 AUTHOR(S): Labadie, Guillermo R.; Cravero, Raquel M.;
 Estiu, Guillermina; Gonzalez Sierra, Manuel
 CORPORATE SOURCE: IQUIOS-Facultad de Cs. Bioquimicas y
 Farmaceuticas, Universidad Nacional de
 Rosario, Santa Fe, 2000, Argent.
 SOURCE: Molecules [Electronic Publication] (2000),
 5(3), 453-454
 CODEN: MOLEFW; ISSN: 1420-3049
 URL: <http://www.mdpi.org/molecules/papers/50300252.pdf>
 PUBLISHER: Molecular Diversity Preservation International
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 AB Birch alkylation products are very unstable. We are showing, in
 this communication, the results of a theor. study that compares
 different decomposition reaction mechanisms. The conclusions are in
 agreement with our exptl. results.
 IT 59034-54-7
 (decomposition mechanism; theor. study of decomposition mechanisms of
 8a-alkyl-1,2,3,4,6,8a-hexahydronaphthalen-1-ones as Birch
 reductive alkylation products of α -tetralone)
 RN 59034-54-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
 (6CI, 9CI) (CA INDEX NAME)

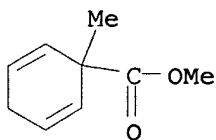


CC 22-7 (Physical Organic Chemistry)
 IT 41477-84-3 59034-54-7 134824-02-5 310897-17-7
 (decomposition mechanism; theor. study of decomposition mechanisms of
 8a-alkyl-1,2,3,4,6,8a-hexahydronaphthalen-1-ones as Birch
 reductive alkylation products of α -tetralone)
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L62 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1996:257738 HCAPLUS
 DOCUMENT NUMBER: 125:11165
 TITLE: A chemoenzymic approach to the taxoid
 BC-substructure
 AUTHOR(S): Arseniyadis, Simeon; Yashunsky, Dmitry V.;
 Munoz Dorado, Manuel; Brondi Alves, Rosemeire;
 Wang, Qian; Potier, Pierre
 CORPORATE SOURCE: Inst. Chim. Subst. Nat., CNRS, Gif-sur-Yvette,
 F-91198, Fr.
 SOURCE: Tetrahedron (1996), 52(17), 6215-32
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 125:11165
 GI



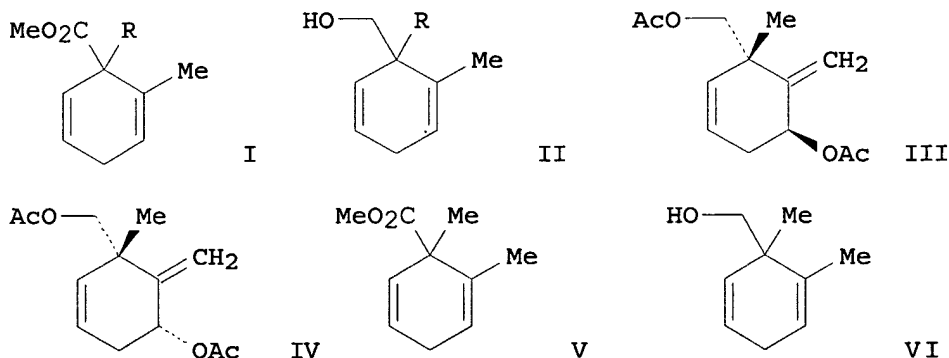
AB The synthesis of homochiral taxoid BC-unit I containing the required
 functionalities on the B-ring periphery and a conveniently
 functionalized C-ring moiety by combination of enzymic hydrolysis
 and the aldol-annulation-fragmentation sequence is described.
 IT 59034-54-7P
 (chemoenzymic approach to the taxoid BC-substructure)
 RN 59034-54-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
 (6CI, 9CI) (CA INDEX NAME)



CC 30-20 (Terpenes and Terpenoids)
 IT 59034-54-7P 72469-77-3P 152455-13-5P 152455-20-4P
 152455-21-5P 152455-23-7P 152455-25-9P 177099-46-6P
 177099-47-7P 177315-29-6P 177315-30-9P 177315-34-3P
 177315-35-4P 177315-36-5P 177315-37-6P 177315-43-4P
 177315-44-5P

(chemoenzymic approach to the taxoid BC-substructure)

L62 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1995:413368 HCAPLUS
 DOCUMENT NUMBER: 123:143069
 TITLE: Substituent Effects in the Highly
 Regioselective and Diastereoselective Ene
 Reaction of Singlet Oxygen with Chiral
 Cyclohexadienes
 AUTHOR(S): Linker, Torsten; Froehlich, Lothar
 CORPORATE SOURCE: Institute of Organic Chemistry, University of
 Wuerzburg, Wuerzburg, D-97074, Germany
 SOURCE: Journal of the American Chemical Society
 (1995), 117(10), 2694-7
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 123:143069
 GI



AB The photooxygenation of the cyclohexadienes I and II, which are readily available through Birch reduction of 2-methylbenzoic acid (1), yielded only one regioisomeric hydroperoxide in a remarkable high diastereoselectivity. A strong directing effect on the stereochem. course of this singlet oxygen ene reaction (Schenk reaction) was observed for various functional groups, including esters and homoallylic alcs. which are unprecedented. This control of diastereoselectivity is rationalized in terms of steric

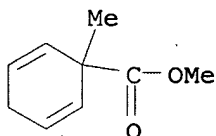
and electronic factors, which provide strong support for peroxide intermediates in the Schenck reaction. An observation important for synthetic applications is the opportunity to steer the attack of 102 by the proper choice of functional groups. Thus, both diacetate diastereomers III and IV were selectively prepared from the ester V or alc. VI of the same starting material 1. The convenience of the reaction sequence Birch reduction-photooxygenation should provide an attractive route to natural products.

IT 59034-54-7

(failed reaction; substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester (6CI, 9CI) (CA INDEX NAME)

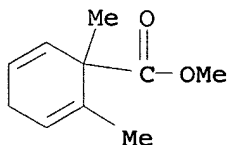


IT 55262-06-1P 55262-07-2P 55262-08-3P

(substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

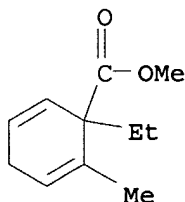
RN 55262-06-1 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1,2-dimethyl-, methyl ester (9CI) (CA INDEX NAME)



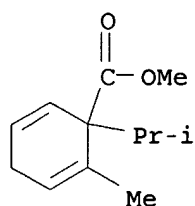
RN 55262-07-2 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-ethyl-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 55262-08-3 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 2-methyl-1-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

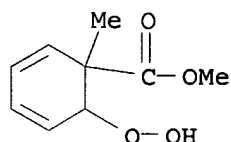


IT 166188-59-6P

(substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

RN 166188-59-6 HCAPLUS

CN 2,4-Cyclohexadiene-1-carboxylic acid, 6-hydroperoxy-1-methyl-, methyl ester (9CI) (CA INDEX NAME)



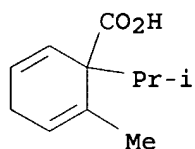
IT 31689-42-6P 55262-10-7P 55262-11-8P

166188-55-2P 166188-56-3P

(substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

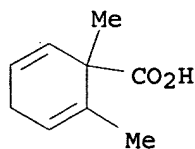
RN 31689-42-6 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 2-methyl-1-(1-methylethyl)- (9CI) (CA INDEX NAME)



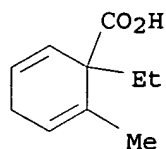
RN 55262-10-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1,2-dimethyl- (9CI) (CA INDEX NAME)



RN 55262-11-8 HCAPLUS

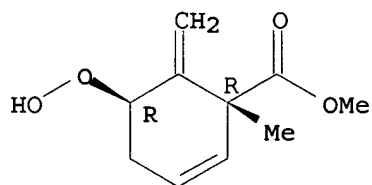
CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-ethyl-2-methyl- (9CI) (CA INDEX NAME)



RN 166188-55-2 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 5-hydroperoxy-1-methyl-6-methylene-, methyl ester, trans- (9CI) (CA INDEX NAME)

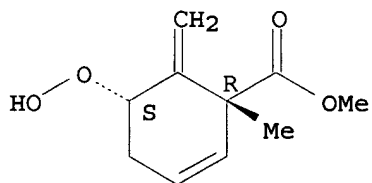
Relative stereochemistry.



RN 166188-56-3 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 5-hydroperoxy-1-methyl-6-methylene-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



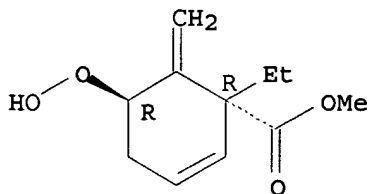
IT 166188-57-4P 166188-58-5P 166188-61-0P

(substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

RN 166188-57-4 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 1-ethyl-5-hydroperoxy-6-methylene-, methyl ester, trans- (9CI) (CA INDEX NAME)

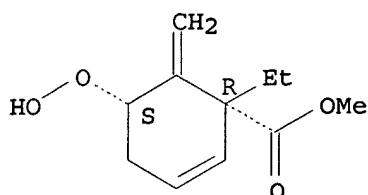
Relative stereochemistry.



RN 166188-58-5 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 1-ethyl-5-hydroperoxy-6-methylene-, methyl ester, cis- (9CI) (CA INDEX NAME)

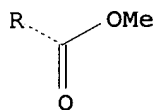
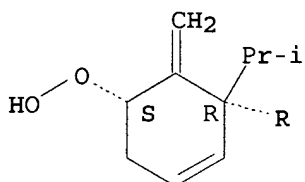
Relative stereochemistry.



RN 166188-61-0 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 5-hydroperoxy-6-methylene-1-(1-methylethyl)-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 22-3 (Physical Organic Chemistry)
Section cross-reference(s): 24, 25

IT 59034-54-7

(failed reaction; substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

IT 55262-06-1P 55262-07-2P 55262-08-3P

166188-51-8P 166188-52-9P 166188-53-0P

(substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

IT 166188-59-6P

(substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

IT 31689-42-6P 55262-10-7P 55262-11-8P

166188-55-2P 166188-56-3P

(substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

IT 144878-61-5P 144939-19-5P 166188-57-4P

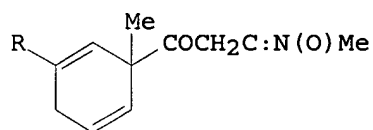
166188-58-5P 166188-60-9P 166188-61-0P

166188-62-1P 166188-63-2P 166188-64-3P 166188-65-4P

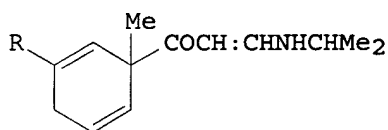
166188-66-5P

(substituent effects in highly regioselective and diastereoselective ene reactions of singlet dioxygen with chiral cyclohexadienes)

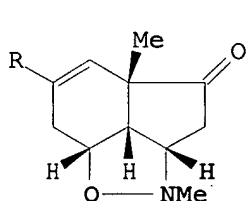
L62 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1988:131091 HCAPLUS
 DOCUMENT NUMBER: 108:131091
 TITLE: Chemoselective intramolecular nitron-olefin
 cycloaddition: an efficient route to
 functionalized cis hydrindane systems
 AUTHOR(S): Stanssens, Dirk; De Keukeleire, Denis;
 Vandewalle, Maurits
 CORPORATE SOURCE: Dep. Org. Chem., State Univ. Gent, Ghent,
 B-9000, Belg.
 SOURCE: Bulletin des Societes Chimiques Belges (1987),
 96(10), 813-20
 CODEN: BSCBAG; ISSN: 0037-9646
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:131091
 GI



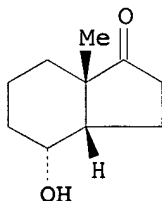
I



II

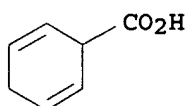


III

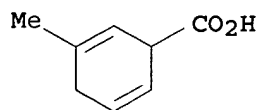


IV

AB Intramol. dipolar [3 + 2]-cycloaddn. of cycloalkenyl oxo nitrones
 I (R = H, Me, MeO), generated in situ from vinylogous amides II
 (same R) and HONHMe.HCl, gives isoxazolidines III regio- and
 stereoselectively. Protection of III (R = H) with HOCH2CH2OH,
 stereoselective reduction, stereoselective hydrogenation, and
 deprotection give hydroxymethylhydrindanone IV.
 IT 4794-04-1, 2,5-Cyclohexadiene-1-carboxylic acid
 31673-44-6 37051-53-9
 (esterification of)
 RN 4794-04-1 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid (6CI, 7CI, 8CI, 9CI) (CA
 INDEX NAME)

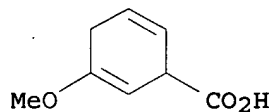


RN 31673-44-6 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 3-methyl- (7CI, 8CI, 9CI)
 (CA INDEX NAME)



RN 37051-53-9 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 3-methoxy- (9CI) (CA INDEX NAME)

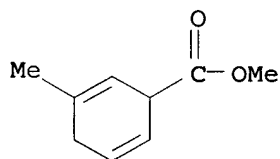


IT 41725-95-5P

(preparation and alkylation of, regiochem. of)

RN 41725-95-5 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 3-methyl-, methyl ester (9CI) (CA INDEX NAME)

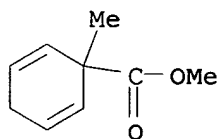


IT 59034-54-7P 82478-18-0P 83766-83-0P

(preparation and homologation of, with ethylideneisopropylamine)

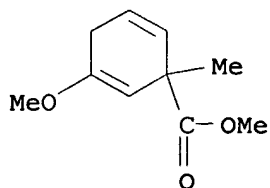
RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester (6CI, 9CI) (CA INDEX NAME)

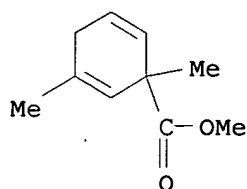


RN 82478-18-0 HCAPLUS

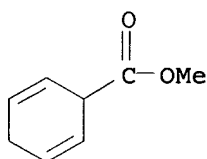
CN 2,5-Cyclohexadiene-1-carboxylic acid, 3-methoxy-1-methyl-, methyl ester (9CI) (CA INDEX NAME)



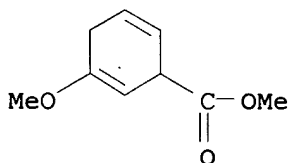
RN 83766-83-0 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1,3-dimethyl-, methyl ester
 (9CI) (CA INDEX NAME)



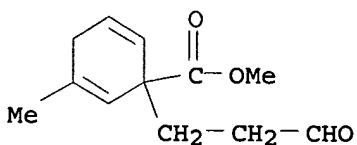
IT 30889-20-4P, Methyl 2,5-cyclohexadiene-1-carboxylate
 113445-19-5P
 (preparation and methylation of, regiochem. of)
 RN 30889-20-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, methyl ester (6CI, 8CI, 9CI)
 (CA INDEX NAME)



RN 113445-19-5 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 3-methoxy-, methyl ester
 (9CI) (CA INDEX NAME)



IT 113445-18-4P
 (preparation, condensation reaction with N-methylhydroxylamine, and
 intramol. cycloaddn. reaction of, stereochem. of)
 RN 113445-18-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 3-methyl-1-(3-oxopropyl)-,
 methyl ester (9CI) (CA INDEX NAME)



CC 24-7 (Alicyclic Compounds)

Section cross-reference(s): 28
 IT 4794-04-1, 2,5-Cyclohexadiene-1-carboxylic acid
 31673-44-6 37051-53-9
 (esterification of)
 IT 41725-95-5P
 (preparation and alkylation of, regiochem. of)
 IT 59034-54-7P 82478-18-0P 83766-83-0P
 (preparation and homologation of, with ethylideneisopropylamine)
 IT 30889-20-4P, Methyl 2,5-cyclohexadiene-1-carboxylate
 113445-19-5P
 (preparation and methylation of, regiochem. of)
 IT 113445-18-4P
 (preparation, condensation reaction with N-methylhydroxylamine, and
 intramol. cycloaddn. reaction of, stereochem. of)

L62 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:55614 HCAPLUS

DOCUMENT NUMBER: 108:55614

TITLE: A synthetically useful conversion of benzoic
 acid derivatives to 4-alkylphenols and
 4-alkyl-3-carbalkoxyphenols

AUTHOR(S): Schultz, Arthur G.; Harrington, Roger E.;
 Macielag, Mark; Mehta, Parag G.; Taveras,
 Arthur G.

CORPORATE SOURCE: Dep. Chem., Rensselaer Polytech. Inst., Troy,
 NY, 12180-3590, USA

SOURCE: Journal of Organic Chemistry (1987), 52(24),
 5482-4

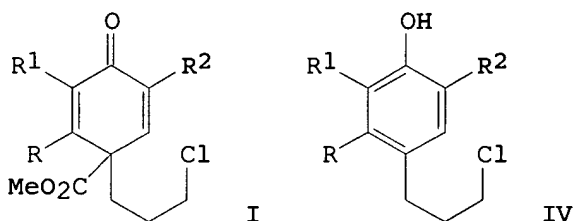
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:55614

GI

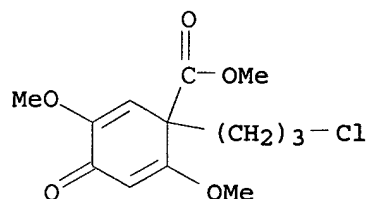


AB 2,5-Cyclohexadien-1-ones I [R, R¹, R² = H, H, H (II); MeO, H, H
 (III); MeO, MeO, H; H, Me, Me] prepared from the corresponding
 benzoic ester by Birch reductive alkylation and allylic oxidation,
 gave 4-(3-chloropropyl)phenols IV (82-89% yields) from treatment
 with 10% NaOH solution at 20°. In a complementary process,
 4-(3-azidopropyl)-2,5-cyclohexadienone, prepared from III via the
 iodopropyl intermediate, gave 78% 2,4-MeO(HO)C₆H₃(CH₂)₃NHCO₂Me on
 treatment with PPh₃ in THF at 20°. II in CF₃CO₂H cleanly
 rearranged to 2,4-MeO₂C(HO)C₆H₃(CH₂)₃Cl.

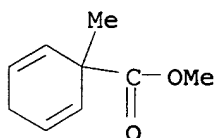
IT 111112-95-9
 (conversion of, to alkylphenol)

RN 111112-95-9 HCAPLUS

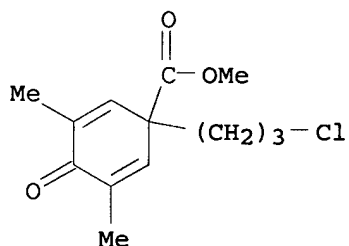
CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(3-chloropropyl)-2,5-
 dimethoxy-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



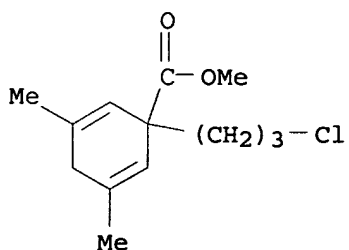
IT 59034-54-7
 (oxidation of)
 RN 59034-54-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
 (6CI, 9CI) (CA INDEX NAME)



IT 111112-93-7P
 (preparation and conversion of, to alkylphenol)
 RN 111112-93-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(3-chloropropyl)-3,5-dimethyl-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

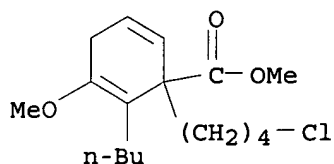


IT 111112-92-6P 111139-84-5P
 (preparation and oxidation of)
 RN 111112-92-6 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(3-chloropropyl)-3,5-dimethyl-, methyl ester (9CI) (CA INDEX NAME)



RN 111139-84-5 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 2-butyl-1-(4-chlorobutyl)-3-methoxy-, methyl ester (9CI) (CA INDEX NAME)

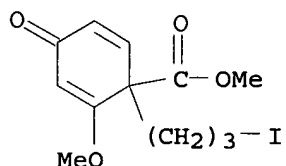


IT 111112-99-3P

(preparation and reaction of, with sodium azide)

RN 111112-99-3 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(3-iodopropyl)-2-methoxy-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

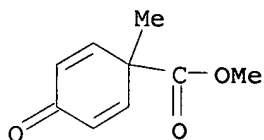


IT 62680-14-2P 111113-04-3P

(preparation and rearrangement of)

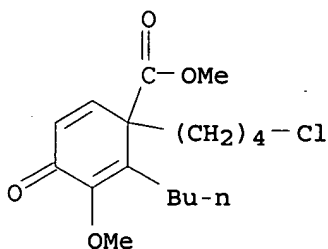
RN 62680-14-2 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 111113-04-3 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 2-butyl-1-(4-chlorobutyl)-3-methoxy-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

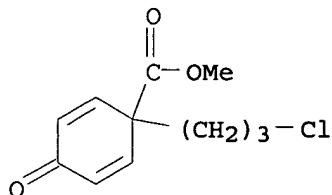


IT 108417-62-5 111112-94-8

(reactions of)

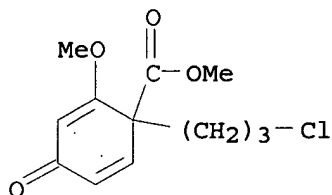
RN 108417-62-5 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(3-chloropropyl)-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 111112-94-8 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(3-chloropropyl)-2-methoxy-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 111112-95-9

(conversion of, to alkylphenol)

IT 59034-54-7

(oxidation of)

IT 111112-93-7P 111113-00-9P

(preparation and conversion of, to alkylphenol)

IT 111112-92-6P 111139-84-5P

(preparation and oxidation of)

IT 111112-99-3P

(preparation and reaction of, with sodium azide)

IT 62680-14-2P 111113-04-3P

(preparation and rearrangement of)

IT 108417-62-5 111112-94-8

(reactions of)

L62 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:552386 HCAPLUS

DOCUMENT NUMBER: 105:152386

TITLE: Novel formation of bis-allylic products by autoxidation of substituted 1,4-cyclohexadienes

AUTHOR(S): Beckwith, A. L. J.; O'Shea, D. M.; Roberts, D. H.

CORPORATE SOURCE: Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia

SOURCE: Journal of the American Chemical Society (1986), 108(20), 6408-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 105:152386

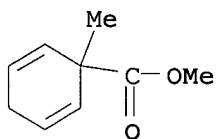
AB Me 1-butyl-2,5-cyclohexadiene-1-carboxylate (I; R = Bu) is stable under N₂; on standing neat in air it gives 35% BzOMe and 65% oxo ester II via the intermediacy of III. III dissociation to PhCO₂Me and Bu• competes with O₂ attack on III to give hydroperoxide IV via the hydroperoxy radical V. The fact that the expected conjugated peroxy radical VI does not give product is due to the rapid equil between V and VI (more rapid than H transfer from I to V or VI) and the steric destabilization of VI relative to V. This destabilization is supported by mol.-mechanics calcns. The mechanism was supported by the ineffective competition of O₂ attack with I (R = PhCH₂) dissociation in air; only BzOMe and PhCH₂OOH were formed.

IT 59034-54-7

(autoxidn. of, mechanism of)

RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester (6CI, 9CI) (CA INDEX NAME)

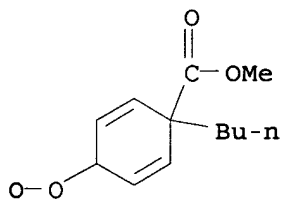


IT 104241-61-4

(isomerization thermodyn. and hydrogen abstraction by)

RN 104241-61-4 HCAPLUS

CN 2,5-Cyclohexadien-1-yldioxy, 4-butyl-4-(methoxycarbonyl)- (9CI) (CA INDEX NAME)

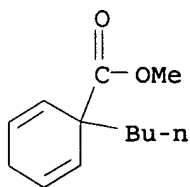


IT 103669-31-4P

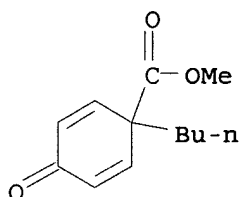
(preparation and autoxidn. of, mechanism and regioselectivity of)

RN 103669-31-4 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-butyl-, methyl ester (9CI) (CA INDEX NAME)



IT 103669-32-5P
 (preparation of)
 RN 103669-32-5 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-butyl-4-oxo-, methyl ester
 (9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)
 IT 59034-54-7 78640-27-4
 (autoxidn. of, mechanism of)
 IT 104241-61-4
 (isomerization thermodyn. and hydrogen abstraction by)
 IT 103669-31-4P
 (preparation and autoxidn. of, mechanism and regioselectivity of)
 IT 103669-32-5P
 (preparation of)

L62 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:34705 HCAPLUS

DOCUMENT NUMBER: 98:34705

TITLE: Organometallic compounds in organic synthesis.
 Part 13. Stereoselectivity of complexation of
 cyclohexadiene esters

AUTHOR(S): Bandara, B. M. Ratnayake; Birch, Arthur J.;
 Raverty, Warwick D.

CORPORATE SOURCE: Res. Sch. Chem., Aust. Natl. Univ., Canberra,
 2600, Australia

SOURCE: Journal of the Chemical Society, Perkin
 Transactions 1: Organic and Bio-Organic
 Chemistry (1972-1999) (1982), (8), 1755-62
 CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

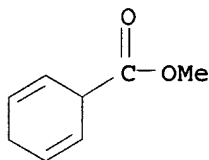
LANGUAGE: English

OTHER SOURCE(S): CASREACT 98:34705

AB The stereochem. of complexation of cyclohexadienes with Fe(CO)₃ as
 the entering group was examined. The reaction was subject to
 classical steric hindrance by alkyl substituents whereas
 alkoxycarbonyl and related groups introduced a competing factor by
 sterically favoring the entering group through formation of an
 intermediate complex. Attachment of OMe groups increased the
 availability of π -electrons in the initial 1,4-diene and
 reduced the influence of the alkoxycarbonyl groups by favoring
 direct olefin complexation. Nonpolar conditions increased the
 directing effects of alkoxycarbonyl groups, but complete
 stereospecificity was achieved only in the presence of addnl.
 alkyl substitution. Many stereoisomeric pairs of products were
 separable to give precursors of various sterically defined
 products not otherwise readily accessible.

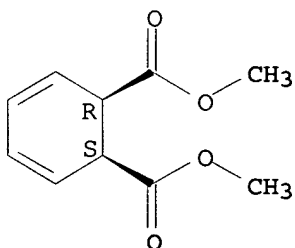
IT 30889-20-4
 (complexation reaction of, with pentacarbonyl iron, stereochem.
 of)

RN 30889-20-4 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, methyl ester (6CI, 8CI, 9CI)
 (CA INDEX NAME)

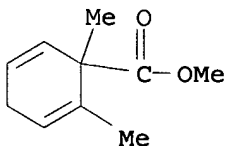


IT 26549-63-3P 55262-06-1P 59034-54-7P
 61040-82-2P 78640-30-9P 83766-83-0P
 83781-11-7P 83781-12-8P
 (preparation and complexation reaction of, with pentacarbonyliron,
 stereochem. of)
 RN 26549-63-3 HCAPLUS
 CN 3,5-Cyclohexadiene-1,2-dicarboxylic acid, dimethyl ester, cis-
 (8CI, 9CI) (CA INDEX NAME)

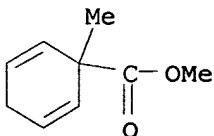
Relative stereochemistry.



RN 55262-06-1 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1,2-dimethyl-, methyl ester
 (9CI) (CA INDEX NAME)

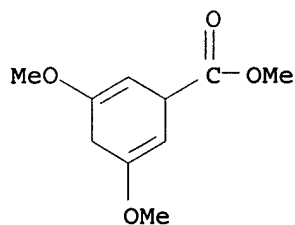


RN 59034-54-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
 (6CI, 9CI) (CA INDEX NAME)



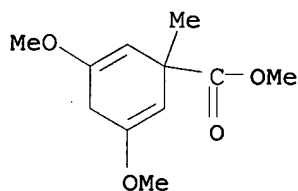
RN 61040-82-2 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 3,5-dimethoxy-, methyl ester
(9CI) (CA INDEX NAME)



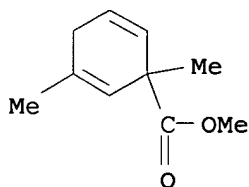
RN 78640-30-9 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 3,5-dimethoxy-1-methyl-,
methyl ester (9CI) (CA INDEX NAME)



RN 83766-83-0 HCAPLUS

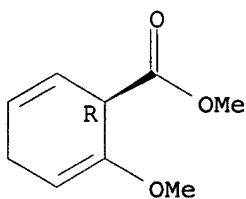
CN 2,5-Cyclohexadiene-1-carboxylic acid, 1,3-dimethyl-, methyl ester
(9CI) (CA INDEX NAME)



RN 83781-11-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 2-methoxy-, methyl ester,
(R) - (9CI) (CA INDEX NAME)

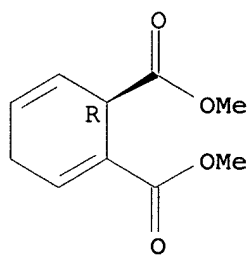
Absolute stereochemistry.



RN 83781-12-8 HCAPLUS

CN 2,5-Cyclohexadiene-1,2-dicarboxylic acid, dimethyl ester, (R) -
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



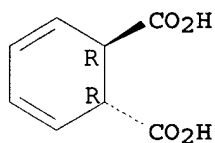
IT 5675-13-8P

(preparation and isomerization of)

RN 5675-13-8 HCAPLUS

CN 3,5-Cyclohexadiene-1,2-dicarboxylic acid, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

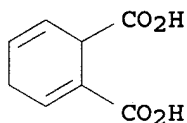


IT 1515-23-7P 55262-10-7P 64286-79-9P

(preparation and methylation of)

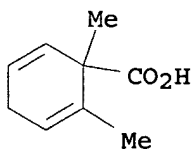
RN 1515-23-7 HCAPLUS

CN 2,5-Cyclohexadiene-1,2-dicarboxylic acid (7CI, 9CI) (CA INDEX NAME)



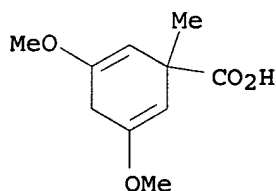
RN 55262-10-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1,2-dimethyl- (9CI) (CA INDEX NAME)



RN 64286-79-9 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 3,5-dimethoxy-1-methyl- (9CI) (CA INDEX NAME)



CC 29-12 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 24

IT 30889-20-4

(complexation reaction of, with pentacarbonyl iron, stereochem. of)

IT 1515-19-1P 26549-63-3P 55262-06-1P

59034-54-7P 61040-82-2P 78640-27-4P

78640-30-9P 83766-80-7P 83766-82-9P

83766-83-0P 83781-11-7P 83781-12-8P

(preparation and complexation reaction of, with pentacarbonyliron, stereochem. of)

IT 5675-13-8P

(preparation and isomerization of)

IT 1515-23-7P 52457-04-2P 55262-10-7P

64286-79-9P

(preparation and methylation of)

L62 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1981:496802 HCAPLUS

DOCUMENT NUMBER: 95:96802

TITLE: Tricarbonyliron complexes of some blocked cyclohexadienes

AUTHOR(S): Bandara, B. M. Ratnayake; Birch, Arthur J.; Chauncy, Brian; Kelly, Lawrence F.

CORPORATE SOURCE: Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia

SOURCE: Journal of Organometallic Chemistry (1981), 208(2), C31-C35

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complexation of substituted 1,3- or 1,4-cyclohexadienes with Fe(CO)₅ indicates that the steric direction is controlled by steric hindrance with groups such as alkyl, but involves transmission of the entering group through intermediate complexation with CO₂Me. The results help to define methods of obtaining desired stereoisomers in the series.

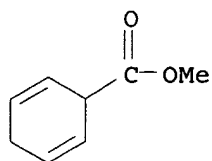
IT 30889-20-4 59034-54-7 78640-25-2

78640-28-5 78640-30-9

(complexation of, with iron pentacarbonyl, stereochem. of)

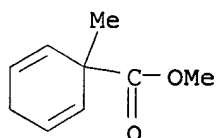
RN 30889-20-4 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, methyl ester (6CI, 8CI, 9CI)
(CA INDEX NAME)



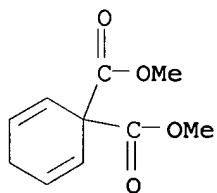
RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
(6CI, 9CI) (CA INDEX NAME)



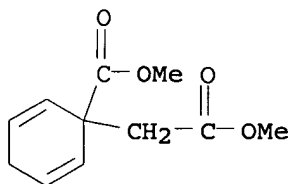
RN 78640-25-2 HCAPLUS

CN 2,5-Cyclohexadiene-1,1-dicarboxylic acid, dimethyl ester (9CI)
(CA INDEX NAME)



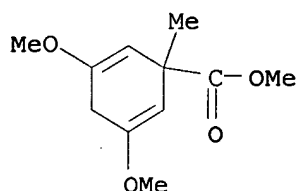
RN 78640-28-5 HCAPLUS

CN 2,5-Cyclohexadiene-1-acetic acid, 1-(methoxycarbonyl)-, methyl ester (9CI) (CA INDEX NAME)



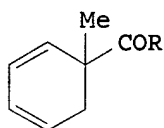
RN 78640-30-9 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 3,5-dimethoxy-1-methyl-, methyl ester (9CI) (CA INDEX NAME)



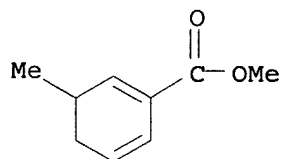
CC 22-9 (Physical Organic Chemistry)
 IT 26592-77-8 30889-20-4 33482-80-3 59034-54-7
 78640-25-2 78640-26-3 78640-27-4 78640-28-5
 78640-29-6 78640-30-9
 (complexation of, with iron pentacarbonyl, stereochem. of)

L62 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1981:479748 HCAPLUS
 DOCUMENT NUMBER: 95:79748
 TITLE: Uncatalyzed sigmatropic 1,5-shift of acyl groups in the thermolysis of 5-acyl-5-methyl-1,3-cyclohexadienes
 AUTHOR(S): Schiess, Peter; Dinkel, Rolf; Fuenfschilling, Peter
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Basel, Basel, 4056, Switz.
 SOURCE: Helvetica Chimica Acta (1981), 64(3), 787-800
 CODEN: HCACAV; ISSN: 0018-019X
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI

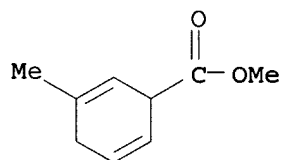


I

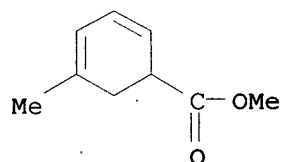
AB Thermolysis of title compds. (I; R = OMe, Me, Ph, H) gave mixts. of 1,3-disubstituted cyclohexadienes and 1,3-disubstituted aromatic product. ¹³C labeling indicated that 75-86% of the product from I (R = OMe) arose via a 1,5-sigmatropic shift of the CO₂Me group and 14-25% arose via a sequence involving a 1,7-H shift in an acyclic intermediate. Isomerizations of I (R = Me, Ph, H) were assumed to follow the 1,5-sigmatropic path exclusively. The migration tendency of the acyl groups via a sigmatropic 1,5-shift increased in the order CO₂Me < COMe < CPh < CHO.
 IT 4134-22-9 41725-95-5 78523-39-4
 78523-40-7
 (IR and NMR spectra of)
 RN 4134-22-9 HCAPLUS
 CN 1,5-Cyclohexadiene-1-carboxylic acid, 3-methyl-, methyl ester
 (7CI, 8CI, 9CI) (CA INDEX NAME)



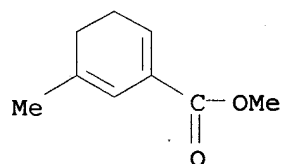
RN 41725-95-5 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 3-methyl-, methyl ester
 (9CI) (CA INDEX NAME)



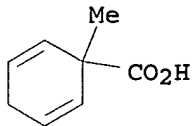
RN 78523-39-4 HCAPLUS
 CN 2,4-Cyclohexadiene-1-carboxylic acid, 5-methyl-, methyl ester
 (9CI) (CA INDEX NAME)



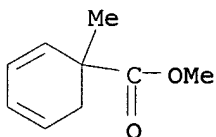
RN 78523-40-7 HCAPLUS
 CN 1,5-Cyclohexadiene-1-carboxylic acid, 5-methyl-, methyl ester
 (9CI) (CA INDEX NAME)



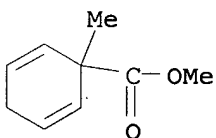
IT 52457-01-9
 (esterification of)
 RN 52457-01-9 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl- (6CI, 9CI) (CA
 INDEX NAME)



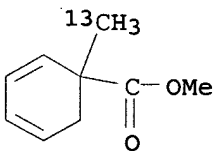
IT 699-42-3
 (isomerization of, mechanism of)
 RN 699-42-3 HCAPLUS
 CN 2,4-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
 (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 59034-54-7P
 (preparation and isomerization of)
 RN 59034-54-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
 (6CI, 9CI) (CA INDEX NAME)



IT 78523-38-3P
 (preparation of)
 RN 78523-38-3 HCAPLUS
 CN 2,4-Cyclohexadiene-1-carboxylic acid, 1-(methyl-13C)-, methyl ester (9CI) (CA INDEX NAME)



CC 22-6 (Physical Organic Chemistry)
 IT 93-58-3 4134-22-9 41725-95-5 51544-58-2
 78523-39-4 78523-40-7 78523-41-8
 (IR and NMR spectra of)
 IT 52457-01-9
 (esterification of)
 IT 699-42-3 40430-79-3 40572-65-4 78523-37-2
 (isomerization of, mechanism of)
 IT 59034-54-7P

(preparation and isomerization of)
 IT 40430-80-6P 78523-38-3P
 (preparation of)

L62 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:214757 HCAPLUS

DOCUMENT NUMBER: 92:214757

TITLE: Stereoselectivity of epoxidation of substituted cyclohexa-1,4-dienes: influence of an allylic methoxycarbonyl group

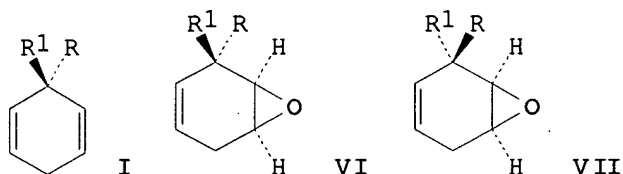
AUTHOR(S): Mah, Talat; Sirat, Hasnah M.; Thomas, Eric J.
 CORPORATE SOURCE: Dep. Chem., King's Coll., London, WC2R 2LS, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1979), (9), 2255-60
 CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Epoxidn. of the dienes I (R = Me, R¹ = CO₂Me, CH₂OH, tetrahydropyranyloxymethyl; R = H, R¹ = CO₂Me) (II-V, resp.) with 3-ClC₆H₄C(O)OOH gave mixts. of the corresponding epoxides VI and VII in which VI was the major component in the mixture from II and III, and VII the major component in the mixture from IV and V. The stereoselectivities are explained in terms of steric hindrance to the approaching peracid; a cis directing effect of the MeO₂C group is not involved. Epoxidn. of Me cis-6-acetoxy-1-methoxycyclohex-2-ene-1-carboxylate gave 9:1 mixture of Me cis-6-acetoxy-1-methylcyclohex-2-ene-1-carboxylate trans- and cis-epoxide.

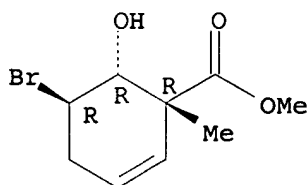
IT 69586-55-6

(epoxide formation from)

RN 69586-55-6 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 5-bromo-6-hydroxy-1-methyl-, methyl ester, (1 α ,5 β ,6 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

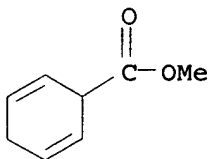


IT 30889-20-4, 59034-54-7

(epoxidn. of, stereochem. of)

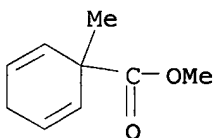
RN 30889-20-4 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, methyl ester (6CI, 8CI, 9CI)
(CA INDEX NAME)



RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
(6CI, 9CI) (CA INDEX NAME)



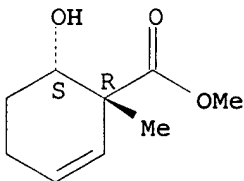
IT 72469-74-0P

(preparation and acetylation of)

RN 72469-74-0 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 6-hydroxy-1-methyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



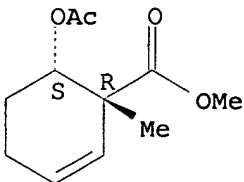
IT 72469-73-9P

(preparation and epoxidn. of, stereochem. of)

RN 72469-73-9 HCAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 6-(acetyloxy)-1-methyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

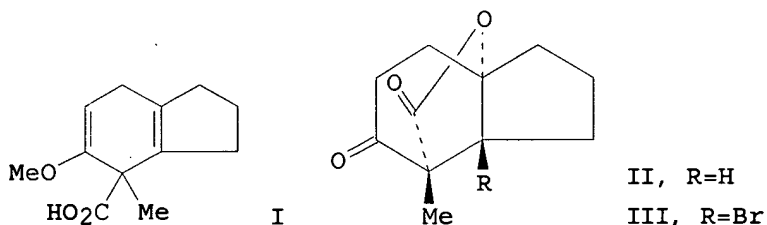


CC 22-9 (Physical Organic Chemistry)

IT 69586-55-6

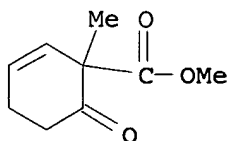
(epoxide formation from)
 IT 30889-20-4 59034-54-7 72469-77-3 72469-79-5
 (epoxidn. of, stereochem. of)
 IT 72469-74-0P
 (preparation and acetylation of)
 IT 72469-73-9P
 (preparation and epoxidn. of, stereochem. of)

L62 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1977:600886 HCAPLUS
 DOCUMENT NUMBER: 87:200886
 TITLE: An efficient synthetic route to a lactone
 model for the gibberellin A ring
 AUTHOR(S): House, Herbert O.; Zaiko, Edward J.
 CORPORATE SOURCE: Sch. Chem., Georgia Inst. Technol., Atlanta,
 GA, USA
 SOURCE: Journal of Organic Chemistry (1977), 42(23),
 3780-3
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

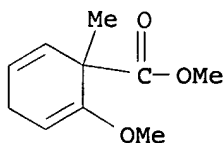


AB The cyclohexadienecarboxylic acid I was converted to the keto
 lactone II by cleavage of the enol ether at -78° with BBr_3 ,
 bromolactonization, and reduction of the bromo lactone III with
 Bu_3SnH .

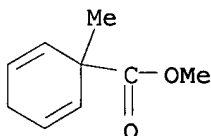
IT 63548-79-8P
 (preparation and epoxidn. of)
 RN 63548-79-8 HCAPLUS
 CN 2-Cyclohexene-1-carboxylic acid, 1-methyl-6-oxo-, methyl ester
 (9CI) (CA INDEX NAME)



IT 21173-69-3P
 (preparation and hydrolysis of)
 RN 21173-69-3 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 2-methoxy-1-methyl-, methyl
 ester (8CI, 9CI) (CA INDEX NAME)

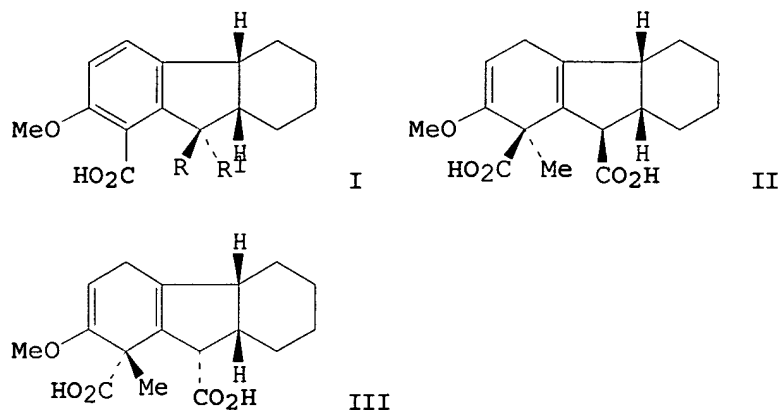


IT 59034-54-7P
 (preparation of)
 RN 59034-54-7 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
 (6CI, 9CI) (CA INDEX NAME)



CC 24-9 (Alicyclic Compounds)
 Section cross-reference(s): 30
 IT 63548-79-8P
 (preparation and epoxidn. of)
 IT 21173-69-3P
 (preparation and hydrolysis of)
 IT 10258-34-1P 59034-54-7P 63548-81-2P 63548-82-3P
 63548-85-6P
 (preparation of)

L62 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1976:446244 HCAPLUS
 DOCUMENT NUMBER: 85:46244
 TITLE: Perhydroindan derivatives. 17. Application
 of the reduction-methylation sequence to
 7-methoxyhexahydrofluorene derivatives
 AUTHOR(S): House, Herbert O.; Strickland, Roger C.;
 Zaiko, Edward J.
 CORPORATE SOURCE: Sch. Chem., Georgia Inst. Technol., Atlanta,
 GA, USA
 SOURCE: Journal of Organic Chemistry (1976), 41(14),
 2401-8
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

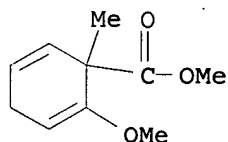


AB The fluorenedicarboxylic acid I (R = CO₂H, R₁ = H) was treated with Li-NH₃ in THF and then with MeI to give II in a stereospecific reaction. III was obtained by the reduction-methylation of I (R = H, R₁ = CO₂H).

IT 21173-69-3P 59034-54-7P
(by reduction-methylation of O-methylsalicylic acid)

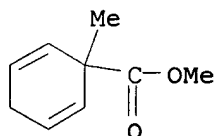
RN 21173-69-3 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 2-methoxy-1-methyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)



RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester (6CI, 9CI) (CA INDEX NAME)



CC 26-4 (Condensed Aromatic Compounds)
Section cross-reference(s): 22

IT 21173-69-3P 59034-54-7P
(by reduction-methylation of O-methylsalicylic acid)

L62 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2006 ACS-on STN

ACCESSION NUMBER: 1961:43196 HCAPLUS

DOCUMENT NUMBER: 55:43196

ORIGINAL REFERENCE NO.: 55:8371a-i,8372a-c

TITLE: Cycloheptatrienes from the solvolysis of 1,4-dihydrobenzyl p-toluenesulfonates

AUTHOR(S): Nelson, Norman A.; Fassnacht, John H.; Piper, James U.

CORPORATE SOURCE: Massachusetts Inst. of Technol., Cambridge

SOURCE: Journal of the American Chemical Society (1961), 83, 206-13

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 55:43196

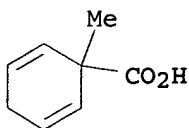
AB The conversion of aromatic carboxylic acids to 1,4-dihydrobenzyl p-toluenesulfonates (I) was described. The solvolysis of the I in AcOH containing NaH₂PO₄ (II) yielded mainly cycloheptatrienes with lesser amts. of esters and aromatic hydrocarbons. Dihydrobenzoic acid (III) (20.5 g.), m. about 10°, in 200 cc. Et₂O added dropwise with stirring to 12.8 g. LiAlH₄ in 400 cc. Et₂O, the mixture refluxed 1 hr., and worked up gave 10.2 g. 1,4-dihydrobenzyl alc. (IV), b₂₀ 95-7°, n_{25D} 1.5043. Crude III (from 30 g. BzOH) reduced directly with 11 g. LiAlH₄ yielded 19.6 g. IV, b₂₀ 94-8°; 3,5-dinitrobenzoate, 81%, m. 89-90.5° (EtOH). IV (4.0 g.) in 100 cc. dry C₅H₅N treated with swirling with 6.8 g. p-MeC₆H₄SO₂Cl (V), the mixture kept 43 hrs. at 0-5°, diluted with Et₂O, and worked up gave 8.7 g. p-toluenesulfonate (VI) of IV, light yellow oil. Crude VI (8.7 g.), 100 cc. AcOH, and 8.9 g. II.H₂O stirred 36 hrs. at 90°, cooled to 0°, neutralized with aqueous NaOH, the product isolated with Et₂O, and chromatographed on 200 g. Al₂O₈ gave 2.1 g. mixture of 12% PhMe and 88% cycloheptatriene (VII) and 0.8 g. crude ester fraction, b₂₀ 130°, which hydrogenated in AcOH over 10% Pd-C gave a mixture of 63% hexahydrobenzyl acetate and 37% cycloheptyl acetate (VIII). VI (22.1 g.) in 300 cc. glacial AcOH heated 40 hrs. at 80° with 16 g. II.H₂O gave 1.3 g. hydrocarbon fraction and 5.3 g. ester fraction, b₁₄₋₁₅ 85-90°; 4.1 g. ester hydrogenated gave 2.7 g. VIII, b. 198-9°. IV (6.0 g.) and 400 mg. KHSO₄ heated 1.5 hrs. at 180-90° yielded 1.2 g. mixed hydrocarbons containing VIII. IV (19.5 g.) and 0.9 g. Dowex-50 resin heated 1 hr. at 175-80° gave 2.8 g. mixture, b. 104-11°, of 25% PhMe, 65% VIII, and 10% minor constituents. KNH₂ from 22.6 g. K and 75 mg. FeCl₃ in 1200 cc. liquid NH₃ treated under N with 34 g. III in 100 cc. Et₂O and after 15 min. with 42 g. MeI during 40 min. and the mixture worked up yielded 34.5 g. crude 1-Me derivative (IX) of III, m. 35-7°, which with CH₂N₂ yielded a mixture of 95% Me ester of IX and 5% BzOMe. Crude IX (28 g.) reduced with 17.1 g. LiAlH₄ gave 15.5 g. 1-Me derivative (X) of IV, b₁₀₀ 105-10°. X (2.1 g.), 2.67 g. p-O₂NC₆H₄CO₂H, and 6.1 g. V in 40 cc. C₅H₅N yielded 3.1 g. p-nitrobenzoate of X, m. 93.5-95° (aqueous EtOH). X (6.6 g.) and 9.9 g. V yielded in the usual manner 13.0 g. crude p-toluenesulfonate (XI) of X, light yellow oil. XI (8.1 g.), 8.5 g. II.H₂O, and 100 cc. AcOH stirred 24 hrs. at 80° yielded 1.6 g. hydrocarbon mixture, b. 135-6°, consisting of 2% unidentified material, 50% 3-Me derivative (XII) of VII, and 48% 1-Me derivative (XIII) of VII; the mixture hydrogenated in AcOH over 10% Pd-C gave methylcycloheptane, n_{27D} 1.4394. III (20 g.) alkylated in the usual manner with 24 g. CD₃I yielded 19.6 g. 1-CD₃ derivative of III which reduced with LiAlH₄ gave 17.0 g. 1-CD₃ derivative (XIV) of IV. XIV (3.3 g.) and 4.6 g. V gave in the usual manner 6.5 g. p-toluenesulfonate (XV) of XIV. XV (6.5 g.) in 80 cc. AcOH heated 36 hrs. at 90° with 6.9 g. II gave 1.8 g. (crude) hydrocarbon mixture, consisting of 2% unidentified material, 50% 3-CD₃ derivative of VII and 48% 1-CD₃ derivative of VII, and 0.85 g.

(crude) ester, b35 105-8°, consisting mainly of the acetate (XVI) of XIV. XIV (1 g.) in 2 g. Ac2O and 1 drop concentrated H2SO4 heated 2 hrs. at 60° and worked up gave 0.75 g. XVI, b35 106-8°, n25D 1.4654. 2-Me derivative (15.9 g.) of III reduced with 9.85 g. LiAlH4 yielded 10.8 g. 2-Me derivative (XVII) of IV, b26 109°, n31D 1.5019. XVII (5.8 g.) with 8.9 g. II gave 8.1 g. p-toluenesulfonate (XVIII) of XVII, m. 42-3° (EtOH). XVIII (12 g.), 12.5 g. II.H2O, and 125 cc. AcOH heated 36 hrs. at 90° gave 3.3 g. mixture of 31% 2-Me derivative (XIX) of VII, 7% XII, 54% XIII, and 8% o-xylene, and 0.90 g. crude ester fraction, which purified by gas chromatography showed the presence of 4% unidentified material, 58% acetate (XX) of XVII, n27D 1.4754, and 38% methylcycloheptadienyl acetate. XVII (1.0 g.) in 2 g. Ac2O and 1 drop C5H5N heated 2.5 hrs. at 80° and worked up gave 0.77 g. XX, b30 115°, n27D 1.4793. XIX (120 mg.), 172 mg. p-MeC6H4SO3H, 300 mg. II.H2O, and 2.5 cc. AcOH heated 12 hrs. with stirring at 90° and worked up gave a mixture of 35% XIX, 14% XII, and 51% XIII. 1,4-Dihydro-1-methyl-1-naphthoic acid (8.0 g.), m. 102-13.5°, reduced with LiAlH4 yielded 7.6 g. (crude) 1,4-dihydro-1-methyl-1-naphthylmethanol (XXI), b0.15 102-4°, containing 3% impurity. XXI (3.4 g.) with 3.8 g. V gave 6.0 g. (crude) p-toluenesulfonate (XXII) of XXI, m. 58-9° (EtOH). XXII (6.0 g.) and 4.6 g. II.H2O in 70 cc. AcOH gave in the usual manner 2.0 g. hydrocarbon mixture, b25 136°, consisting of 1,2-benzo-3-methylcycloheptatriene and 1,2-benzo-4-methylcycloheptatriene with 3% unidentified material and 0.19 g. ester fraction. Hydrocarbon mixture (from XXII) (0.50 g.) in 5 cc. AcOH hydrogenated over 75 mg. 10% Pd-C gave 0.48 g. product consisting of 15% unidentified hydrocarbon, presumably 1,2-benzo-4-methylcycloheptene, and 85% 1,2-benzo-3-methylcycloheptene (XXIII). MeMgI from 5.2 g. MeI and 0.86 g. Mg in 40 cc. Et2O treated with stirring with 5 g. benzosuberone in 20 cc. Et2O, the mixture worked up, and the product heated on the steam bath with 50% H2SO4 gave 5 g. crude olefin, b30 128°; a 0.5-g. portion hydrogenated catalytically gave 0.5 g. XXIII.

IT 52457-01-9, 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl- 59034-54-7, 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester 98752-35-3, 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-d3- (preparation of)

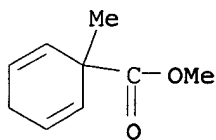
RN 52457-01-9 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl- (6CI, 9CI) (CA INDEX NAME)

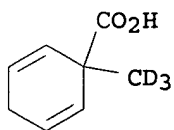


RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester (6CI, 9CI) (CA INDEX NAME)



RN 98752-35-3 HCAPLUS
 CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(methyl-d3)- (6CI, 9CI)
 (CA INDEX NAME)



CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)
 IT 937-55-3, Cyclohexanemethanol, acetate 3045-88-3,
 1,3,5-Cycloheptatriene, 1-methyl- 3045-89-4,
 1,3,5-Cycloheptatriene, 2-methyl- 3045-90-7,
 1,3,5-Cycloheptatriene, 3-methyl- 18631-70-4, Cycloheptanol,
 acetate 22851-69-0, 5H-Benzocycloheptene, 6,7,8,9-tetrahydro-6-
 methyl- 25372-69-4, 2,5-Cyclohexadiene-1-methanol
 52457-01-9, 2,5-Cyclohexadiene-1-carboxylic acid,
 1-methyl- 59034-54-7, 2,5-Cyclohexadiene-1-carboxylic
 acid, 1-methyl-, methyl ester 72469-77-3, 2,5-Cyclohexadiene-1-
 methanol, 1-methyl- 98752-35-3, 2,5-Cyclohexadiene-1-
 carboxylic acid, 1-methyl-d3- 101654-27-7, 2,5-Cyclohexadiene-1-
 methanol, 2-methyl- 102171-94-8, 1-Naphthalenemethanol,
 1,4-dihydro-1-methyl-, p-toluenesulfonate 104851-38-9,
 5H-Benzocycloheptene, 6,7,8,9-tetrahydro-5-methyl- 105695-73-6,
 1-Naphthalenemethanol, 1,4-dihydro-1-methyl- 117273-23-1,
 Cycloheptadieneacetic acid, methyl ester 118873-04-4,
 2,5-Cyclohexadiene-1-methanol, 1-methyl-d3- 122238-67-9,
 1,3,5-Cycloheptatriene, 3-methyl-d3- 122238-68-0,
 1,3,5-Cycloheptatriene, 1-methyl-d3-
 (preparation of)

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L11 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:165012 HCAPLUS Full-text

DOCUMENT NUMBER: 142:429810

TITLE: 1,4-Cyclohexadienes as mechanistic probes for the Jacobsen epoxidation: evidence for radical pathways

AUTHOR(S): Engelhardt, Ulrike; Linker, Torsten

CORPORATE SOURCE: Department of Chemistry, University of Potsdam, Potsdam, D-14476, Germany

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (9), 1152-1154

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:429810

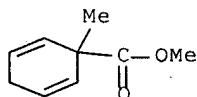
AB 1,4-Cyclohexadienes allow a direct comparison of epoxidn. and C-H oxidation within the same mol. and give evidence for radical pathways during the Jacobsen epoxidn.

IT 59034-54-7

(uncatalyzed epoxidn. and catalyzed allylic oxidation; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)

RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester (6CI, 9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)

IT Oxidation catalysts

(allylic oxidation of 1,4-cyclohexadienes using Jacobsen epoxidn. catalyst; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)

IT Oxidation

(allylic, of 1,4-cyclohexadienes using Jacobsen epoxidn. catalyst; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)

IT Reaction mechanism

(radical; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)

IT Epoxidation

(uncatalyzed epoxidn. of 1,4-cyclohexadienes with MCPBA; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)

IT 138124-32-0, (R,R)-Jacobsen's catalyst

((R,R)-Jacobsen's catalyst; 1,4-cyclohexadienes as mechanistic

probes for the Jacobsen epoxidn. provide evidence for radical pathways)

- IT 62680-14-2P 119711-72-7P 131236-66-3P 849116-59-2P
849116-60-5P
(1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)
- IT 7529-22-8, N-Methylmorpholine N-oxide
(co-ligand; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)
- IT 849116-58-1P
(dr = 57:43; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)
- IT 849116-57-0P
(dr = 65:35; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)
- IT 849116-56-9P
(dr = 76:24; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)
- IT 937-14-4, MCPBA
(stoichiometric oxidant; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)
- IT 55262-06-1 59034-54-7 83766-83-0
(uncatalyzed epoxidn. and catalyzed allylic oxidation; 1,4-cyclohexadienes as mechanistic probes for the Jacobsen epoxidn. provide evidence for radical pathways)

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:799884 HCAPLUS Full-text

DOCUMENT NUMBER: 136:53451

TITLE: Homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids: an EPR spectroscopic study of chain propagation

AUTHOR(S): Jackson, Leon V.; Walton, John C.

CORPORATE SOURCE: School of Chemistry, University of St. Andrews, St. Andrews, KY16 9ST, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 2 (2001), (9), 1758-1764
CODEN: JCSPGI; ISSN: 1472-779X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:53451

AB Hydrogen abstraction from 1-substituted cyclohexa-2,5-diene-1-carboxylic acids containing linear, branched and cyclic alkyl substituents, as well as allyl, propargyl (prop-2-ynyl), cyanomethyl and benzyl substituents, has been studied by EPR spectroscopy. For each carboxylic acid, EPR spectra of the corresponding cyclohexadienyl radicals were observed at lower temps., followed by spectra due to ejected carbon-centered radicals at higher temps. Rate consts., for release of the carbon-centered radicals from the cyclohexadienyl radicals, were determined from radical concentration measurements for the above range of substituents. The rate of cyclohexadienyl radical dissociation increased with branching in the 1-alkyl substituent and with electron

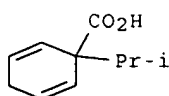
delocalization in the ejected carbon-centered radical; 3,5- and 2,6-dimethyl-substitution of the cyclohexadienyl ring led to redns. in the dissociation rate consts. Rate data for abstraction of bis allylic hydrogens from the cyclohexadienyl acids were also obtained for Et, Pr and iso-Pr radicals. These results indicated a sharp drop in the rate of hydrogen abstraction as the degree of branching in the attacking radical increased. Small decreases in the hydrogen abstraction rate consts. were observed for cyclohexadienes containing CO₂R substituents.

IT 31689-39-1

(H abstraction by tert-butoxy; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids)

RN 31689-39-1 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1-methylethyl)- (9CI)
(CA INDEX NAME)

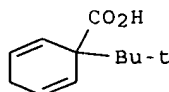


IT 52457-02-0P 52457-04-2P 245672-30-4P
380883-30-7P

(H abstraction by tert-butoxy; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids)

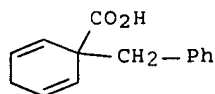
RN 52457-02-0 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)



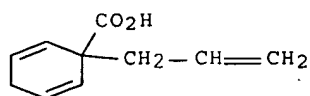
RN 52457-04-2 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(phenylmethyl)- (9CI) (CA INDEX NAME)



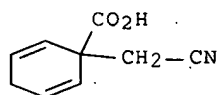
RN 245672-30-4 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(2-propenyl)- (9CI) (CA INDEX NAME)



RN 380883-30-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(cyanomethyl)- (9CI) (CA
INDEX NAME)



CC 22-8 (Physical Organic Chemistry)

IT Radicals, reactions

(cyclohexadienyl and alkyl; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids)

IT Resonance

(in cyclohexadienyl radical dissociation fragment; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids)

IT ESR (electron spin resonance)

(of cyclohexadienyl and alkyl radicals; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids)

IT Dissociation

(of cyclohexadienyl radicals in chain mechanism; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids)

IT AM1 (molecular orbital method)

Conformation

Dissociation enthalpy

Dissociation kinetics

Formation enthalpy

Hyperfine coupling

Molecular structure

(of cyclohexadienyl radicals; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids)

IT 31689-39-1 52457-01-9 52457-03-1 380883-31-8

(H abstraction by tert-butoxy; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted cyclohexa-2,5-diene-1-carboxylic acids)

IT 31689-38-0P 31689-40-4P 52457-02-0P

52457-04-2P 245672-30-4P 380883-28-3P

380883-29-4P 380883-30-7P 380883-32-9P 380883-33-0P

380883-34-1P 380883-36-3P

(H abstraction by tert-butoxy; ESR spectroscopic study of chain propagation in the homolytic dissociation of 1-substituted

cyclohexa-2,5-diene-1-carboxylic acids)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

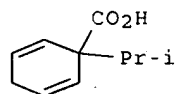
L11 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:589481 HCAPLUS Full-text
DOCUMENT NUMBER: 131:299212
TITLE: The efficiency of alkyl radical
generation and hydrogen transfer from
1-alkylcyclohexa-2,5-diene-1-carboxylic acids
AUTHOR(S): Jackson, Leon; Walton, John C.
CORPORATE SOURCE: School of Chemistry, University of St.
Andrews, St. Andrews, Fife, KY16 9ST, UK
SOURCE: Tetrahedron Letters (1999), 40(38), 7019-7021
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel ESR spectroscopic technique was used to determine kinetic data for
alkyl-radical generation and H transfer from 1-alkyl-2,5-cyclohexadiene-1-
carboxylic acids. The implications of these data for preparative chain
reactions of these reagents are inferred.

IT 31689-39-1, 2,5-Cyclohexadiene-1-carboxylic acid,
1-(1-methylethyl)- 52457-02-0, 2,5-Cyclohexadiene-1-
carboxylic acid, 1-(1,1-dimethylethyl)-
(efficiency of alkyl-radical generation and hydrogen
transfer from alkylcyclohexadienecarboxylic acids)

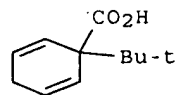
RN 31689-39-1 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1-methylethyl)- (9CI)
(CA INDEX NAME)



RN 52457-02-0 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)



CC 22-10 (Physical Organic Chemistry)

IT Activation energy
Decomposition kinetics
ESR (electron spin resonance)
Hydrogen transfer kinetics
Stabilization energy
(efficiency of alkyl-radical generation and hydrogen

transfer from alkylcyclohexadienecarboxylic acids)
 IT Radicals, formation (nonpreparative)
 (efficiency of alkyl-radical generation and hydrogen
 transfer from alkylcyclohexadienecarboxylic acids)
 IT Abstraction reaction kinetics
 (hydrogen; efficiency of alkyl-radical generation and
 hydrogen transfer from alkylcyclohexadienecarboxylic acids)
 IT 31689-38-0, 2,5-Cyclohexadiene-1-carboxylic acid, 1-ethyl-
 31689-39-1, 2,5-Cyclohexadiene-1-carboxylic acid,
 1-(1-methylethyl)- 31689-40-4 52457-01-9, 1-Methyl-2,5-
 cyclohexadiene-1-carboxylic acid 52457-02-0,
 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1,1-dimethylethyl)-
 (efficiency of alkyl-radical generation and hydrogen
 transfer from alkylcyclohexadienecarboxylic acids)
 REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L11 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1998:429845 HCAPLUS Full-text
 DOCUMENT NUMBER: 129:175370
 TITLE: Reductive free-radical alkylation
 and cyclization mediated by
 1-alkyl-2,5-cyclohexadiene-1-carboxylic acids
 AUTHOR(S): Baguley, Paul A.; Walton, John C.
 CORPORATE SOURCE: School of Chemistry, University of St.
 Andrews, St. Andrews, KY16 9ST, UK
 SOURCE: Journal of the Chemical Society, Perkin
 Transactions 1: Organic and Bio-Organic
 Chemistry (1998), (13), 2073-2082
 CODEN: JCPRB4; ISSN: 0300-922X
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 129:175370

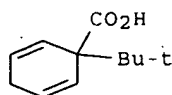
AB A range of 1-alkyl-2,5-cyclohexadiene-1-carboxylic acids were prepared by Birch
 reduction-alkylation of benzoic acid and their efficiency as mediators of
 alkyl radical chain addition and cyclization processes was investigated.
 Reductive alkylation were respectably successful, even with only one or two
 equivalent of alkene, for secondary, tertiary and benzylic radicals. Reaction
 of 1-[2-(cyclohex-2-enyloxy)ethyl]-2,5-cyclohexadiene-1-carboxylic acid
 yielded the product of exo-trig-cyclization, i.e. 7-oxabicyclo[4.3.0]nonane,
 in a yield comparable to that obtained from the tributyltin hydride induced
 cyclization of 3-(2'-iodoethoxy)cyclohexene. This, together with the
 isolation of both exo- and endo-cyclization products from 1-[2-(6,6-
 dimethylbicyclo[3.1.1]hept-2-en-2-ylmethoxy)ethyl]-2,5-cyclohexadiene-1-
 carboxylic acid established that ring closures could also be satisfactorily
 mediated with these reagents. Preps. were completely free of metal
 contaminants and direct reduction of the alkyl radicals, prior to addition or
 cyclization, was completely absent. However, the desired products were
 accompanied by alkylbenzenes, together with byproducts from the initiator
 decomps., this complicated work-up. Failure to obtain 1-[2-(prop-2-yn-1-
 yloxy)cyclohexyl]-2,5-cyclohexadiene-1-carboxylic acid in Birch reductive
 alkylation with trans-1-iodo-2-(prop-2-yn-1-yloxy)cyclohexane (and the
 corresponding bromide) indicated a limitation on precursor synthesis. The
 Birch reduction-alkylation was not of universal applicability and was
 suppressed for alkyl halides having β -substituents.

IT 52457-02-0P 52457-04-2P
 (preparation of alkylcyclohexadienecarboxylates and their use in
 reductive radical alkylation and cyclization

reactions)

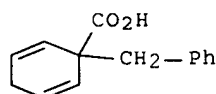
RN 52457-02-0 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)



RN 52457-04-2 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(phenylmethyl)- (9CI) (CA
INDEX NAME)



CC 24-5 (Alicyclic Compounds)

Section cross-reference(s): 22

ST reductive radical alkylation cyclization
alkylcyclohexadienecarboxylate

IT Alkenes, reactions

(preparation of alkylcyclohexadienecarboxylates and their use in
reductive radical alkylation and cyclization
reactions)

IT Addition reaction

(radical; preparation of alkylcyclohexadienecarboxylates
and their use in reductive radical alkylation and
cyclization reactions)

IT Alkylation

Cyclization

(reductive, radical; preparation of
alkylcyclohexadienecarboxylates and their use in reductive
radical alkylation and cyclization reactions)

IT 92-52-4P, Biphenyl, preparation 98-06-6P, tert-Butylbenzene
700-88-9P, Phenylcyclopentane

(preparation of alkylcyclohexadienecarboxylates and their use in
reductive radical alkylation and cyclization
reactions)

IT 65-85-0, Benzoic acid, reactions 100-44-7, Benzyl chloride,
reactions 107-13-1, 2-Propenenitrile, reactions 107-19-7,
Propargyl alcohol 107-21-1, 1,2-Ethanediol, reactions

110-83-8, Cyclohexene, reactions 127-91-3, β -Pinene

137-43-9, Bromocyclopentane 507-19-7, tert-Butyl bromide

540-51-2, 2-Bromoethanol 769-78-8, Vinyl benzoate 930-68-7,

2-Cyclohexen-1-one 1521-51-3, 3-Bromo-1-cyclohexene

120368-06-1

(preparation of alkylcyclohexadienecarboxylates and their use in
reductive radical alkylation and cyclization
reactions)

IT 17140-74-8P 22339-11-3P 52457-02-0P 52457-03-1P

52457-04-2P 90112-73-5P 112701-86-7P 133625-64-6P
183808-73-3P 183808-75-5P 211365-62-7P 211365-63-8P
211365-68-3P 211365-70-7P 211365-71-8P

(preparation of alkylcyclohexadienecarboxylates and their use in
reductive radical alkylation and cyclization
reactions)

IT 936-99-2P 1123-04-2P, Cyclopentanepropanenitrile 27608-11-3P
85450-51-7P 211365-69-4P

(preparation of alkylcyclohexadienecarboxylates and their use in
reductive radical alkylation and cyclization
reactions)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L11 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:618038 HCAPLUS Full-text

DOCUMENT NUMBER: 126:7559

TITLE: Unique carbon-carbon bond homolysis in
3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid
radicals

AUTHOR(S): Baguley, Paul A.; Binmore, Gavin; Milne,
Aynsley; Walton, John C.

CORPORATE SOURCE: Sch. of Chem., Univ. of St. Andrews, St.
Andrews, Fife, KY16 9ST, UK

SOURCE: Chemical Communications (Cambridge) (1996),
(18), 2199-2200

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

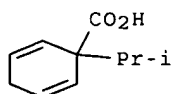
AB 3-Substituted cyclohexadienyl radicals generated by hydrogen abstraction from
3-alkylcyclohexa-1,4-diene-3-carboxylic acids readily fragment to produce
alkyl radicals and benzoic acid; suitably functionalized alkyl groups cyclize
in moderate yields.

IT 31689-39-1 52457-02-0

(precursor; generation of cyclohexadienyl radicals by
hydrogen abstraction from cyclohexadienecarboxylic acid)

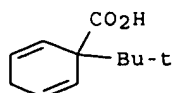
RN 31689-39-1 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1-methylethyl)- (9CI)
(CA INDEX NAME)



RN 52457-02-0 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)



CC 22-6 (Physical Organic Chemistry)

ST alkylcyclohexadienylcarboxylic acid radicals formation
homolysis

IT Cyclization
Cyclization kinetics
(carbon-carbon bond homolysis in 3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals)

IT Radicals, reactions
(carbon-carbon bond homolysis in 3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals)

IT Bond cleavage
(carbon-carbon; carbon-carbon bond homolysis in
3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals
)

IT Abstraction reaction
Abstraction reaction kinetics
(hydrogen; carbon-carbon bond homolysis in 3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals)

IT 16183-00-9, 5-Hexenyl 23907-66-6 183808-77-7 183808-78-8
183905-99-9
(carbon-carbon bond homolysis in 3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals)

IT 96-37-7P, Methylcyclopentane 592-41-6P, 1-Hexene, preparation
13054-97-2P
(carbon-carbon bond homolysis in 3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals)

IT 98-06-6, tert-Butylbenzene 700-88-9, Cyclopentylbenzene
2564-86-5
(cyclohexadienyl acids as radical sources in chain
reactions designed for synthetic purposes)

IT 107-13-1, 2-Propenenitrile, reactions 769-78-8, Vinyl benzoate
930-68-7, 2-Cyclohexen-1-one
(cyclohexadienyl acids as radical sources in chain
reactions designed for synthetic purposes)

IT 936-99-2P 27608-11-3P
(cyclohexadienyl acids as radical sources in chain
reactions designed for synthetic purposes)

IT 1605-73-8, tert-Butyl radical 183905-96-6
183905-97-7 183905-98-8
(generation of cyclohexadienyl radicals by hydrogen
abstraction from cyclohexadienecarboxylic acid)

IT 183808-72-2
(intermediate; cyclohexadienyl acids as radical
sources in chain reactions designed for synthetic purposes)

IT 183808-79-9
(precursor; carbon-carbon bond homolysis in
3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals
)

IT 183808-75-5P
(precursor; carbon-carbon bond homolysis in
3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals
)

IT 31689-38-0 31689-39-1 52457-01-9, 1-Methyl-2,5-cyclohexadiene-1-carboxylic acid 52457-02-0
(precursor; generation of cyclohexadienyl radicals by
hydrogen abstraction from cyclohexadienecarboxylic acid)

IT 183808-73-3

(starting material; carbon-carbon bond homolysis in
3-alkylcyclohexa-1,4-dienyl-3-carboxylic acid radicals
)

L11 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:552386 HCAPLUS Full-text

DOCUMENT NUMBER: 105:152386

TITLE: Novel formation of bis-allylic products by
autoxidation of substituted
1,4-cyclohexadienes

AUTHOR(S): Beckwith, A. L. J.; O'Shea, D. M.; Roberts, D.
H.

CORPORATE SOURCE: Res. Sch. Chem., Aust. Natl. Univ., Canberra,
2601, Australia

SOURCE: Journal of the American Chemical Society
(1986), 108(20), 6408-9
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 105:152386

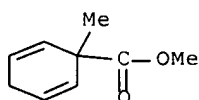
AB Me 1-butyl-2,5-cyclohexadiene-1-carboxylate (I; R = Bu) is stable under N₂; on
standing neat in air it gives 35% BzOMe and 65% oxo ester II via the
intermediacy of III. III dissociation to PhCO₂Me and Bu• competes with O₂
attack on III to give hydroperoxide IV via the hydroperoxy radical V. The
fact that the expected conjugated peroxy radical VI does not give product is
due to the rapid equil between V and VI (more rapid than H transfer from I to
V or VI) and the steric destabilization of VI relative to V. This
destabilization is supported by mol.-mechanics calcns. The mechanism was
supported by the ineffective competition of O₂ attack with I (R = PhCH₂)
dissociation in air; only BzOMe and PhCH₂OOH were formed.

IT 59034-54-7

(autoxidn. of, mechanism of)

RN 59034-54-7 HCAPLUS

CN 2,5-Cyclohexadiene-1-carboxylic acid, 1-methyl-, methyl ester
(6CI, 9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)

IT Conformation and Conformers
(of cyclohexadienes and their derived radicals)

IT Electron spin resonance
(of cyclohexadienyl radical derivative)

IT Coupling reaction
(of cyclohexadienyl radicals with dioxygen)

IT Dissociation
(of cyclohexadienyl radical)

IT 59034-54-7 78640-27-4
(autoxidn. of, mechanism of)

IT 68072-62-8
(of cyclohexadienyl radical derivative)